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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	3	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	4	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	5	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	6	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	7	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	8	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	9	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	10	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	11	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	12	JUN 25	CA/CAPplus and USPAT databases updated with IPC reclassification data
NEWS	13	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS	14	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS	15	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS	16	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS	17	JUL 28	CA/CAPplus patent coverage enhanced
NEWS	18	JUL 28	EPFULL enhanced with additional legal status information from the epline Register
NEWS	19	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	20	JUL 28	STN Viewer performance improved
NEWS	21	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	22	AUG 13	CA/CAPplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	23	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	24	AUG 15	CAPplus currency for Korean patents enhanced
NEWS	25	AUG 25	CA/CAPplus, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching
NEWS	26	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 19:00:00 ON 14 SEP 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 19:00:10 ON 14 SEP 2008
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 SEP 2008 HIGHEST RN 1049105-01-2
DICTIONARY FILE UPDATES: 12 SEP 2008 HIGHEST RN 1049105-01-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

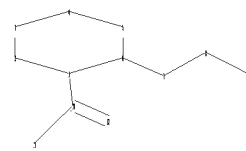
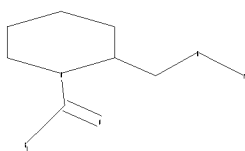
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10527833\Struc 1.str



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chain nodes :
7 8 9 10 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
1-10 6-7 7-8 8-9 10-11 10-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-10 2-3 3-4 4-5 5-6 7-8 8-9 10-11 10-12
exact bonds :
6-7

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G1:Cb,Cy,Hy

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

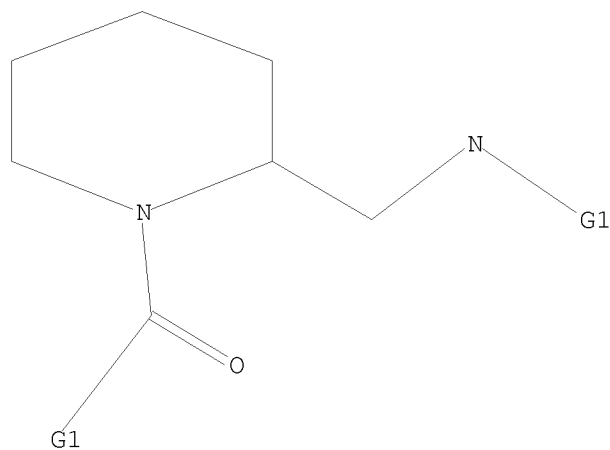
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> l1

SAMPLE SEARCH INITIATED 19:00:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 27849 TO ITERATE

7.2% PROCESSED 2000 ITERATIONS

7 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 546996 TO 566964

PROJECTED ANSWERS: 1357 TO 2541

L2 7 SEA SSS SAM L1

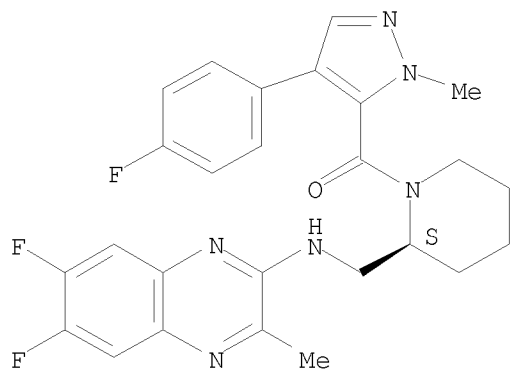
=> d scan

L2 7 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Methanone, [(2S)-2-[[[(6,7-difluoro-3-methyl-2-quinoxalinyloxy)amino]methyl]-1-piperidinyl]][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-5-yl]-

MF C26 H25 F3 N6 O

Absolute stereochemistry.

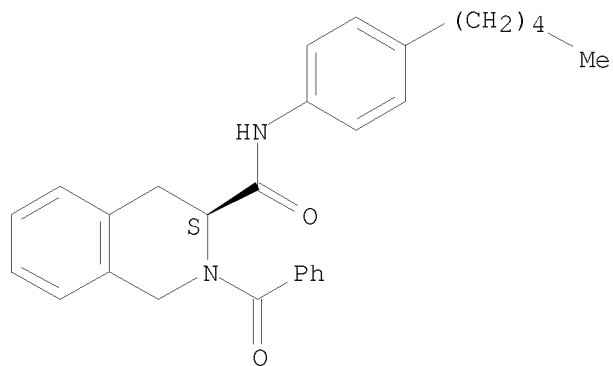


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

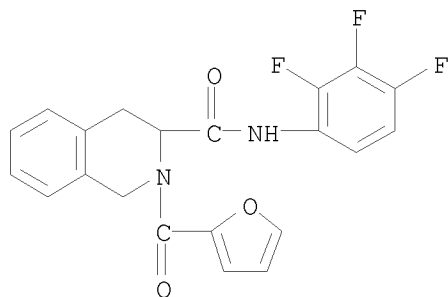
L2 7 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 3-Isoquinolinecarboxamide, 2-benzoyl-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-
 , (3S)-
 MF C28 H30 N2 O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 7 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 3-Isoquinolinecarboxamide, 2-(2-furanylcarbonyl)-1,2,3,4-tetrahydro-N-
 (2,3,4-trifluorophenyl)-
 MF C21 H15 F3 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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FULL SEARCH INITIATED 19:02:52 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 556658 TO ITERATE

99.6% PROCESSED	554243 ITERATIONS	1180 ANSWERS
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100.0% PROCESSED	556658 ITERATIONS	1180 ANSWERS
SEARCH TIME: 00.00.18		

L3 1180 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	180.66	180.87

FILE 'CAPLUS' ENTERED AT 19:03:29 ON 14 SEP 2008

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FILE COVERS 1907 - 14 Sep 2008 VOL 149 ISS 12

FILE LAST UPDATED: 12 Sep 2008 (20080912/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

10527833.trn

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> 13

L4 36 L3

=> d ibib abs hitstr 1-36

L4 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:832909 CAPLUS

DOCUMENT NUMBER: 149:152935

TITLE: 2-Azabicyclo[3.1.0]hexane derivatives as orexin
receptor antagonists and their preparation,
pharmaceutical compositions and use in the treatment
of diseases

INVENTOR(S): Aissaoui, Hamed; Boss, Christoph; Gude, Markus;
Koberstein, Ralf; Sifferlen, Thierry; Trachsel, Daniel

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd., Switz.

SOURCE: PCT Int. Appl., 168pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

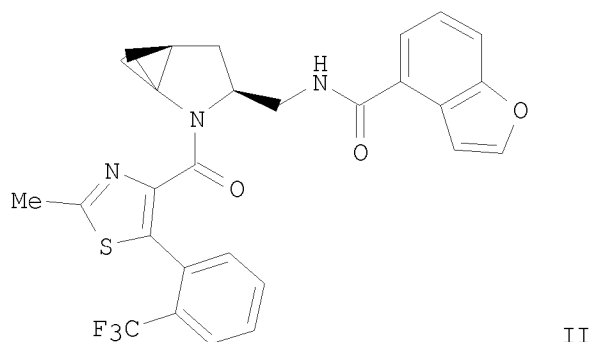
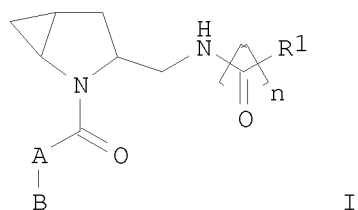
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008081399	A2	20080710	WO 2007-IB55326	20071228
WO 2008081399	A3	20080828		
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

PRIORITY APPLN. INFO.: WO 2006-IB55042 A 20061228

OTHER SOURCE(S): MARPAT 149:152935

GI



AB The invention relates to 2-azabicyclo[3.1.0]hexane derivs. of formula I, and to the use of such compds., or of pharmaceutically acceptable salts of such compds., as medicaments, especially as orexin receptor antagonists. Compds. of formula I wherein A, B and R1 are independently (un)substituted aryl and (un)substituted heterocyclyl; n is 0 and 1; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their orexin receptor antagonistic activity (some data given).

IT 1038508-45-0P 1038508-46-1P 1038508-47-2P
 1038508-48-3P 1038508-49-4P 1038508-50-7P
 1038508-51-8P 1038508-52-9P 1038508-53-0P
 1038508-54-1P 1038508-55-2P 1038508-56-3P
 1038508-57-4P 1038508-58-5P 1038508-59-6P
 1038508-60-9P 1038508-61-0P 1038508-62-1P
 1038508-63-2P 1038508-64-3P 1038508-65-4P
 1038508-66-5P 1038508-67-6P 1038508-68-7P
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 1038508-72-3P 1038508-73-4P

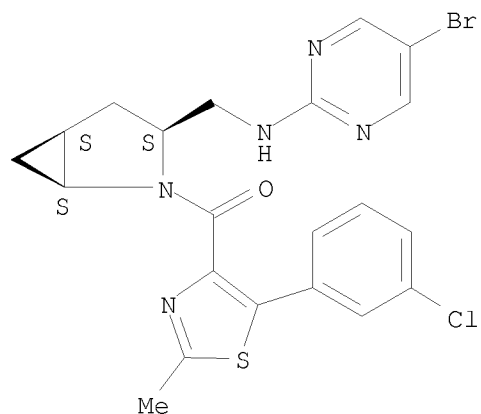
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of azabicyclohexane derivs. as orexin receptor antagonists useful in treatment and prevention of diseases)

RN 1038508-45-0 CAPLUS

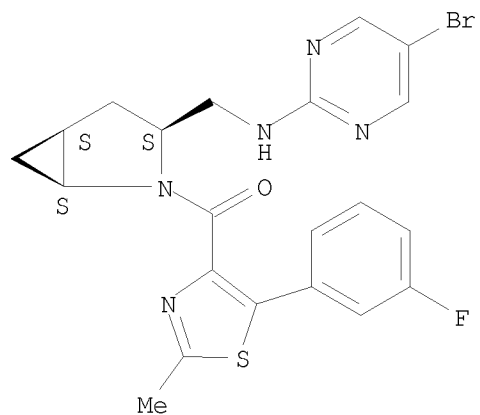
CN Methanone, [(1S,3S,5S)-3-[[(5-bromo-2-pyrimidinyl)amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][5-(3-chlorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



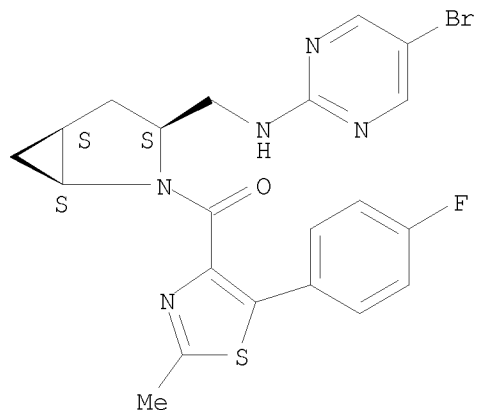
RN 1038508-46-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



RN 1038508-47-2 CAPLUS
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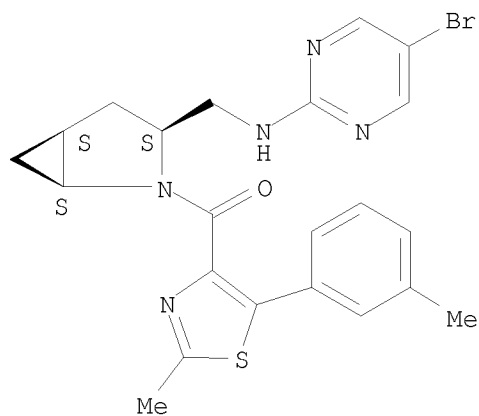
Absolute stereochemistry.



RN 1038508-48-3 CAPLUS

CN Methanone, [(1S,3S,5S)-3-[[5-bromo-2-pyrimidinyl]amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][2-methyl-5-(3-methylphenyl)-4-thiazolyl]- (CA INDEX NAME)

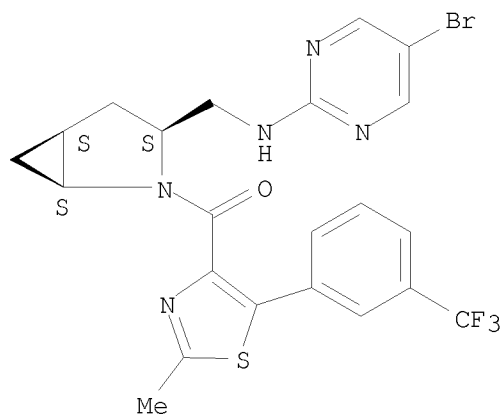
Absolute stereochemistry.



RN 1038508-49-4 CAPLUS

CN Methanone, [(1S,3S,5S)-3-[[5-bromo-2-pyrimidinyl]amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][2-methyl-5-[3-(trifluoromethyl)phenyl]-4-thiazolyl]- (CA INDEX NAME)

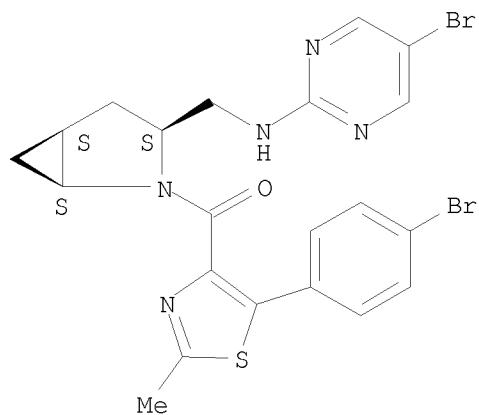
Absolute stereochemistry.



RN 1038508-50-7 CAPLUS

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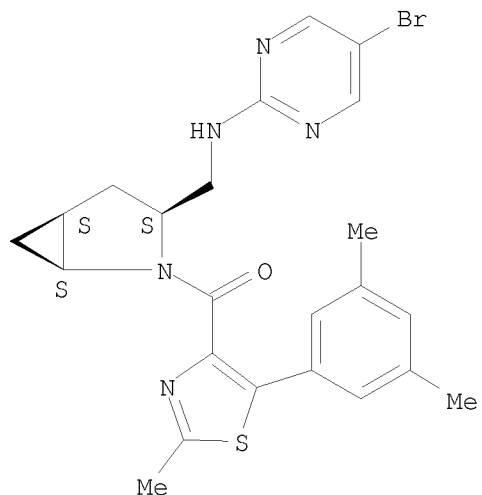
Absolute stereochemistry.



RN 1038508-51-8 CAPLUS

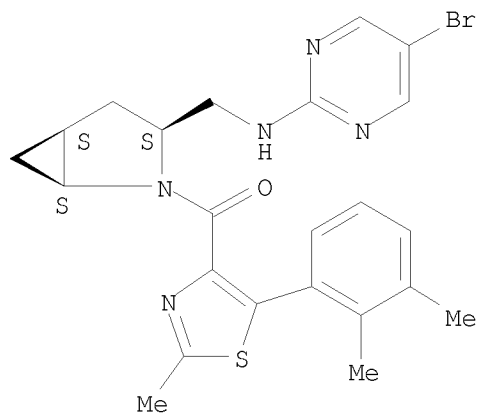
CN Methanone, [(1S,3S,5S)-3-[[5-bromo-2-pyrimidinyl)amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][5-(3,5-dimethylphenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



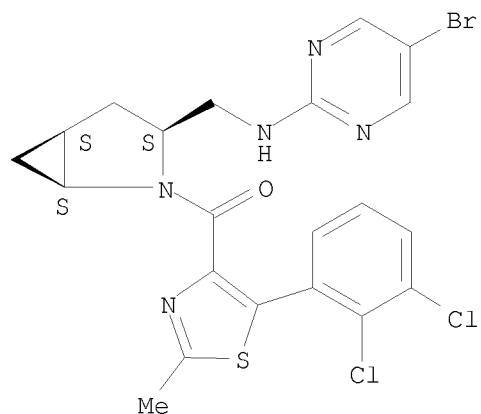
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 (CA INDEX NAME)

Absolute stereochemistry.



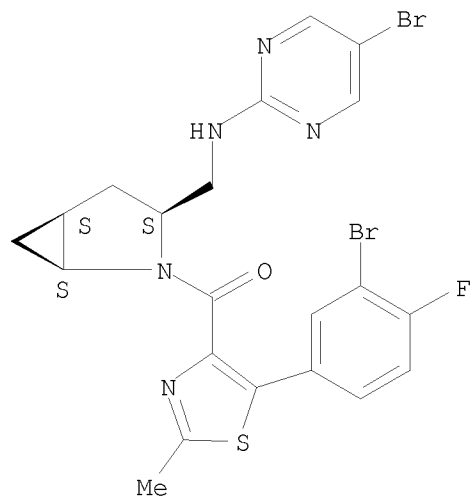
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 (CA INDEX NAME)

Absolute stereochemistry.



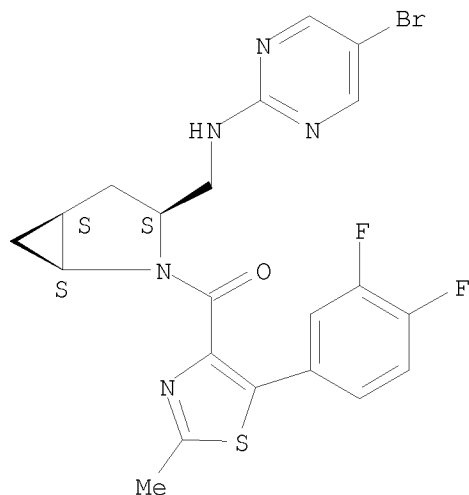
RN 1038508-54-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



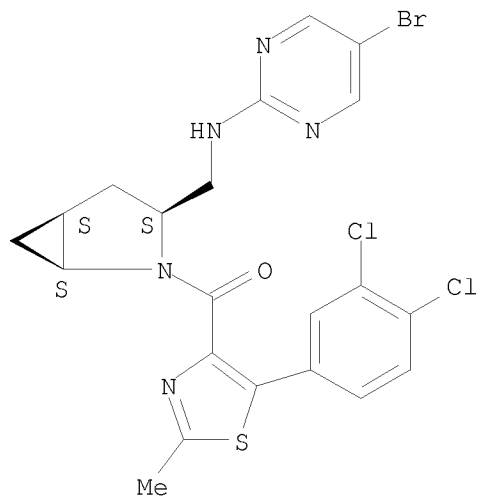
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(CA INDEX NAME)

Absolute stereochemistry.



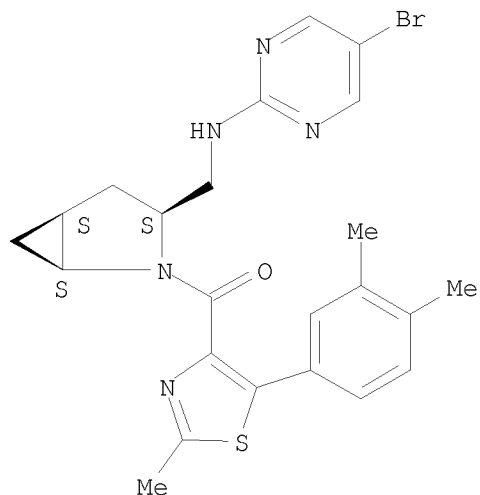
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 (CA INDEX NAME)

Absolute stereochemistry.



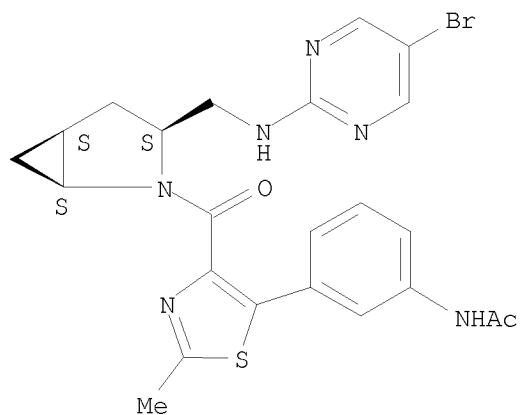
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 (CA INDEX NAME)

Absolute stereochemistry.



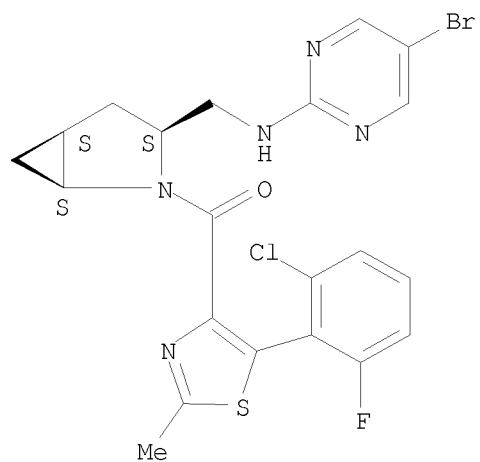
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Absolute stereochemistry.



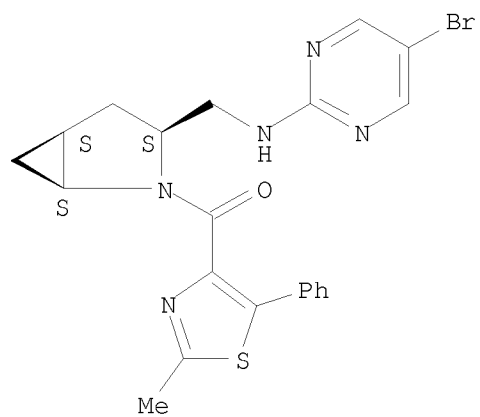
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Absolute stereochemistry.



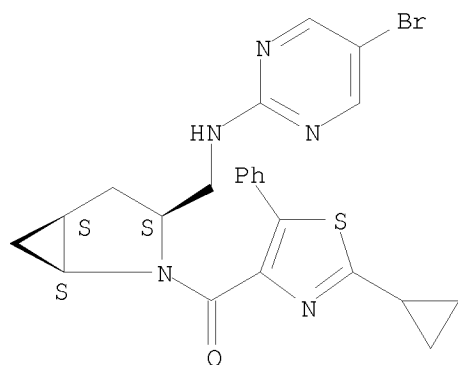
RN 1038508-60-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



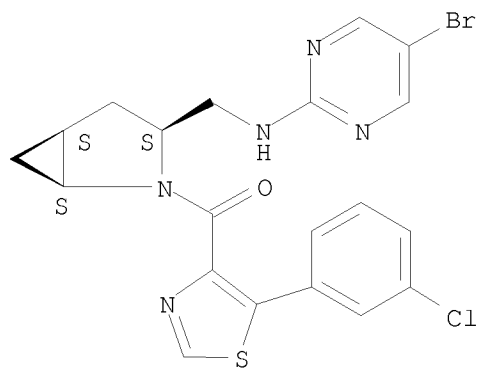
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Absolute stereochemistry.



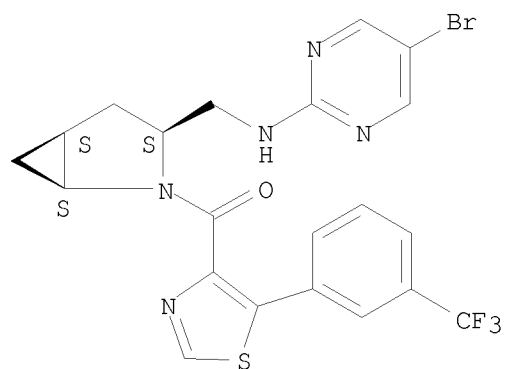
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Absolute stereochemistry.



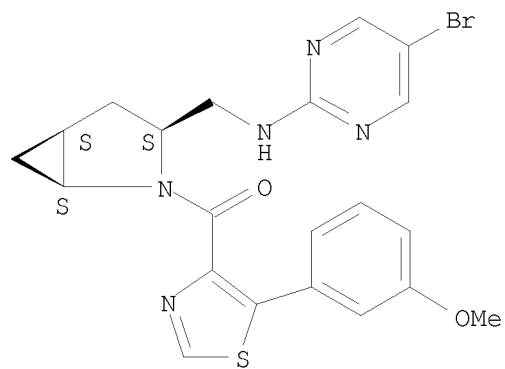
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 CN Methanone, [(1S,3S,5S)-3-[[5-bromo-2-pyrimidinyl)amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][5-[3-(trifluoromethyl)phenyl]-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



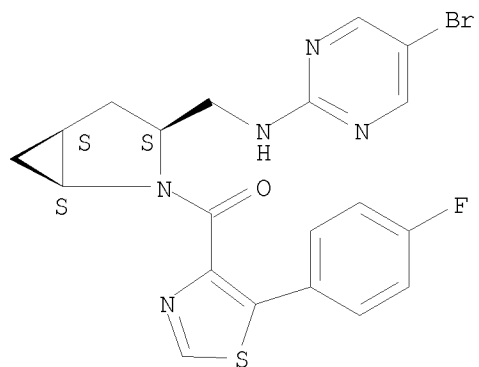
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Absolute stereochemistry.



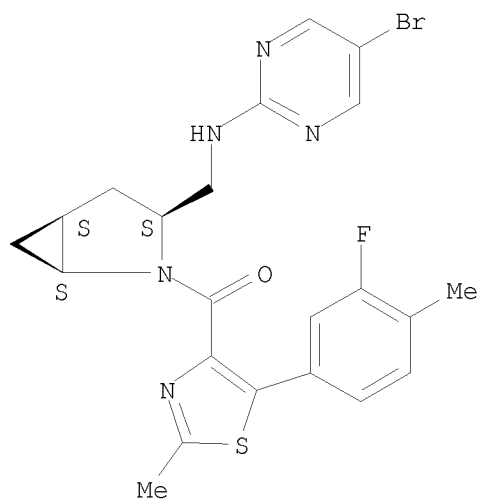
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 CN Methanone, [(1S,3S,5S)-3-[[5-bromo-2-pyrimidinyl)amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][5-(4-fluorophenyl)-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



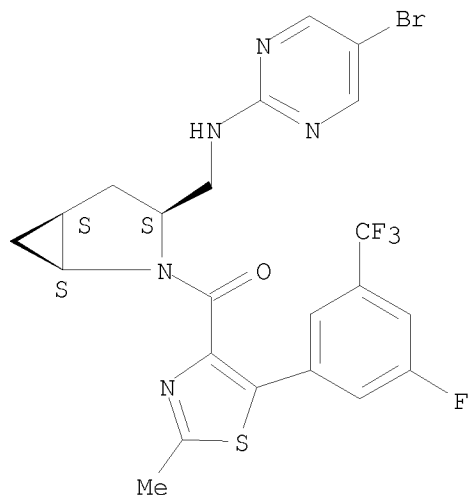
RN 1038508-66-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



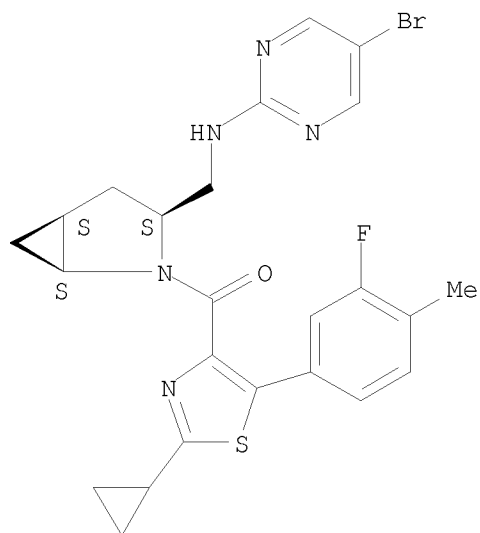
RN 1038508-67-6 CAPLUS
CN Methanone, [(1S,3S,5S)-3-[[5-bromo-2-pyrimidinyl]amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][5-[3-fluoro-5-(trifluoromethyl)phenyl]-2-methyl-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



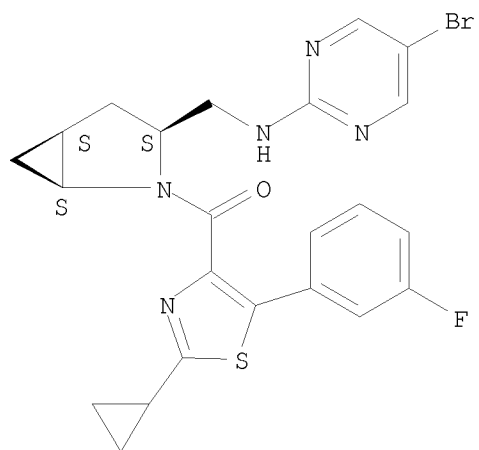
RN 1038508-68-7 CAPLUS
 CN Methanone, [(1S,3S,5S)-3-[[(5-bromo-2-pyrimidinyl)amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][2-cyclopropyl-5-(3-fluoro-4-methylphenyl)-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



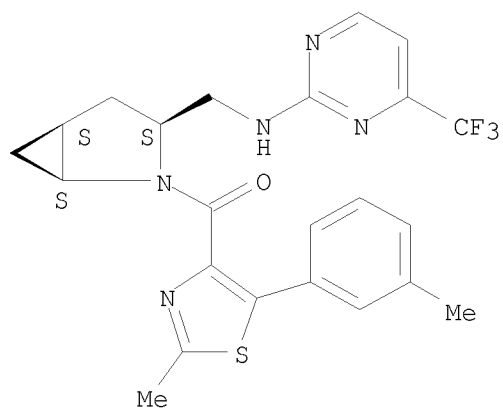
RN 1038508-69-8 CAPLUS
 CN Methanone, [(1S,3S,5S)-3-[[(5-bromo-2-pyrimidinyl)amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][2-cyclopropyl-5-(3-fluorophenyl)-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



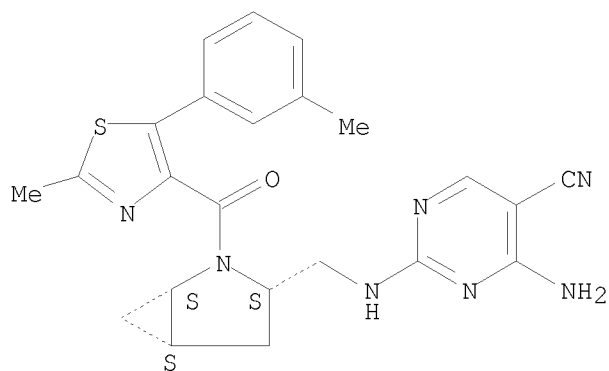
RN 1038508-70-1 CAPLUS
 CN Methanone, [2-methyl-5-(3-methylphenyl)-4-thiazolyl][(1S,3S,5S)-3-[[[4-(trifluoromethyl)-2-pyrimidinyl]amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl]]-(CA INDEX NAME)

Absolute stereochemistry.



RN 1038508-71-2 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

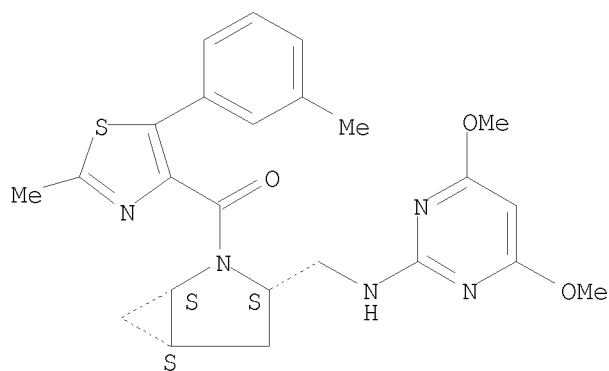
Absolute stereochemistry.



RN 1038508-72-3 CAPLUS

CN Methanone, [(1S,3S,5S)-3-[[[4,6-dimethoxy-2-pyrimidinyl]amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][2-methyl-5-(3-methylphenyl)-4-thiazolyl]- (CA INDEX NAME)

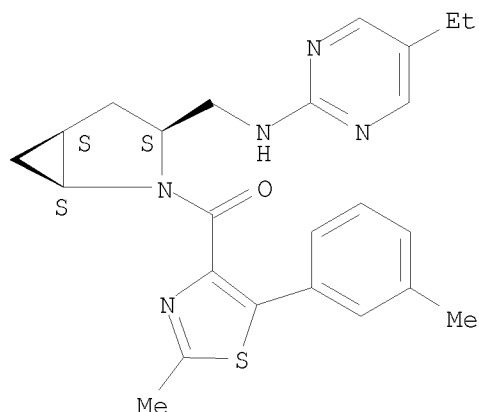
Absolute stereochemistry.



RN 1038508-73-4 CAPLUS

CN Methanone, [(1S,3S,5S)-3-[[[5-ethyl-2-pyrimidinyl]amino]methyl]-2-azabicyclo[3.1.0]hex-2-yl][2-methyl-5-(3-methylphenyl)-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:504901 CAPLUS

DOCUMENT NUMBER: 148:496349

TITLE: Preparation of aryl substituted pyrazoles, especially N-[4-[[1H-pyrazol-4-yl]ethynyl]phenyl]dipeptide derivatives, as HCV antiviral agents and their use in the treatment of hepatitis C infection

INVENTOR(S): Li, Guolin; Fathi, Reza; Yang, Zhen; Liao, Yun; Zhu, Qiang; Lam, Angela; Sandrasagra, Anthony; Nawoschik, Kenneth; Cho, Hyun-Joon; Cao, Jie; Ruoqiu, Wu; Wobbe, C. Richard

PATENT ASSIGNEE(S): XTL Biopharmaceuticals Ltd, USA

SOURCE: PCT Int. Appl., 131pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

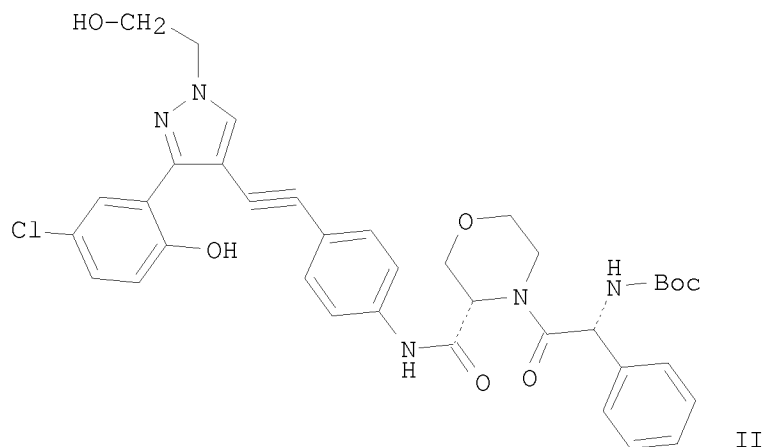
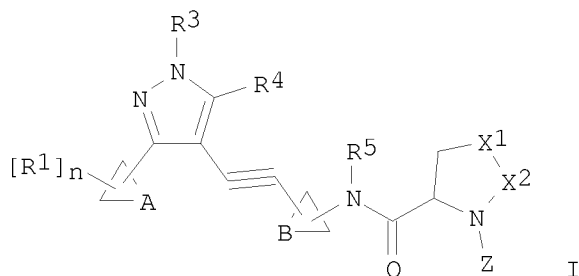
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008048589	A2	20080424	WO 2007-US22055	20071015
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.:
 US 2006-851643P P 20061013
 US 2007-925528P P 20070420
 US 2007-933565P P 20070606

OTHER SOURCE(S): MARPAT 148:496349

GI



AB The invention is related to the preparation of aryl substituted pyrazole derivs. I [A, B = independently 5-6 membered aromatic ring optionally containing 0-3 ring heteroatoms; R1 = independently at each occurrence alk(en/yn)yl, aralkyl, CN, CF3, SO2, halo, etc.; or 2 of R1 may be combined to form an (un)substituted 5-6 fused membered ring optionally containing 0-3 ring heteroatoms; R3 = H, cycloalk(en)yl, aryl, heterocyclyl, etc.; R4 = H, CN, CF3, aryl, cycloalkyl, alkenyl, etc.; R5 = H, alkyl, cycloalkenyl, heterocyclyl, etc.; X1 = CH2, O, S, SO2, NH and derivs.; X2 = CH2, CH2CH2, COCH2, CO; Z = H, alk(en/yn)yl, cycloalkenyl, heterocyclyl, SO2H and derivs.; or Z = ABCR8; A = CH2, SO2; B = (CH2)mCHR6(CH2)p, (un)substituted cyclopropylidene, etc.; m, p = independently 0-4; R6 = H, cycloalkyl, aryl, etc.; R8 = H, aralkyl, NH2, aminoalkyl, alkyl, aryl, etc.; q = 0-6] and their pharmaceutically acceptable salts and hydrates as HCV antiviral agents. The invention is also related to compns. and methods for the treatment of HCV by administering a compound of the present invention, alone or in combination with addnl. antiviral agents, in a therapeutically effective amount. Thus, II was prepared by a multi-step synthesis via peptide coupling using 6-chloro-3-iodochromone, 4-ethynylaniline, (S)-morpholine-3,4-dicarboxylic acid 4-tert-Bu ester and N-(tert-butoxycarbonyl)-D-phenylglycine. The invention compds. were tested in the replicon inhibition luciferase assay, replicon inhibition RNA assay and cell viability assay for the HCV genotype 1b.

IT 1020841-08-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

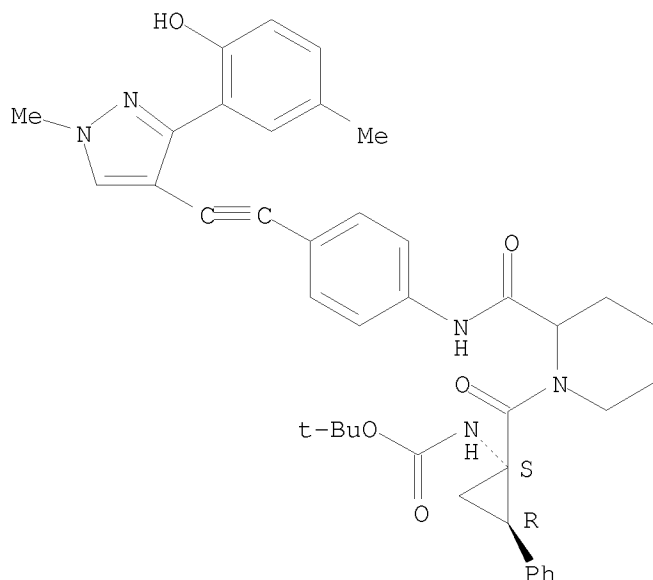
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aryl substituted pyrazoles, especially N-[4-[[1H-pyrazol-4-yl]ethynyl]phenyl]dipeptide derivs., and their use in treatment of hepatitis C infection)

RN 1020841-08-0 CAPLUS

CN Carbamic acid, N-[(1S,2R)-1-[[2-[[[4-[2-[3-(2-hydroxy-5-methylphenyl)-1-methyl-1H-pyrazol-4-yl]ethynyl]phenyl]amino]carbonyl]-1-piperidinyl]carbonyl]-2-phenylcyclopropyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:417764 CAPLUS

DOCUMENT NUMBER: 148:426739

TITLE: 3-Azabicyclo[3.1.0]hexane derivatives as orexin receptor antagonists and their preparation, pharmaceutical compositions and use in the treatment of diseases

INVENTOR(S): Aissaoui, Hamed; Boss, Christoph; Gude, Markus; Koberstein, Ralf; Lehmann, David; Sifferlen, Thierry; Trachsel, Daniel

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd., Switz.

SOURCE: PCT Int. Appl., 209pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008038251	A2	20080403	WO 2007-IB53947	20070928

WO 2008038251

A3

20080626

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.:

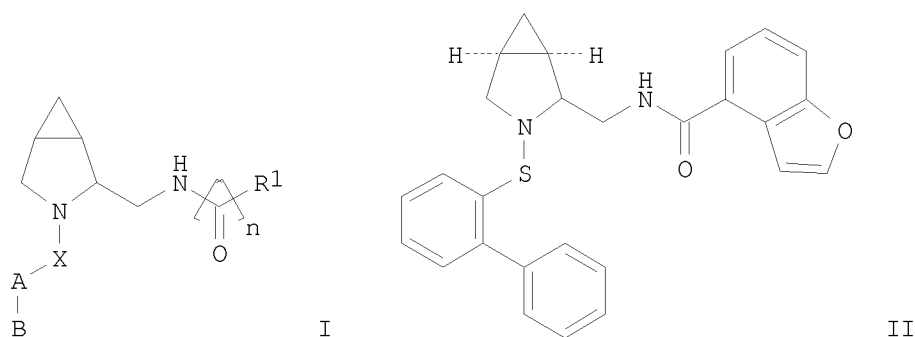
WO 2006-IB53570

A 20060929

OTHER SOURCE(S):

MARPAT 148:426739

GI



AB The invention relates to 3-aza-bicyclo[3.1.0]hexane derivs. of formula I and salts thereof, and their use as orexin receptor antagonists. Comps. of formula I wherein X is CO and SO₂; A is (un)substituted aryl and (un)substituted heterocyclyl; B is H, (un)substituted aryl and (un)substituted heteroaryl; A and B together is tricyclic group; R₁ is (un)substituted aryl and (un)substituted heteroaryl; n is 0 and 1; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by sulfonylation of benzofuran-4-carboxylic acid with [(1R*,2S*,5S*)-3-azabicyclo[3.1.0]hex-2-ylmethyl]amide with biphenyl-2-sulfonyl chloride. All the invention comps. were evaluated for their orexin receptor antagonistic activity (some data given).

IT 1017267-04-7P 1017267-05-8P 1017267-06-9P

1017267-07-0P 1017267-08-1P 1017267-09-2P

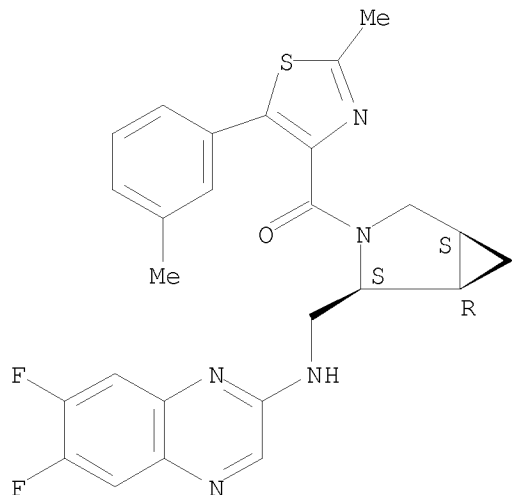
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of azabicyclohexane derivs. as orexin receptor antagonists)

RN 1017267-04-7 CAPLUS

CN Methanone, [(1R,2S,5S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-3-azabicyclo[3.1.0]hex-3-yl][2-methyl-5-(3-methylphenyl)-4-thiazolyl]-, rel- (CA INDEX NAME)

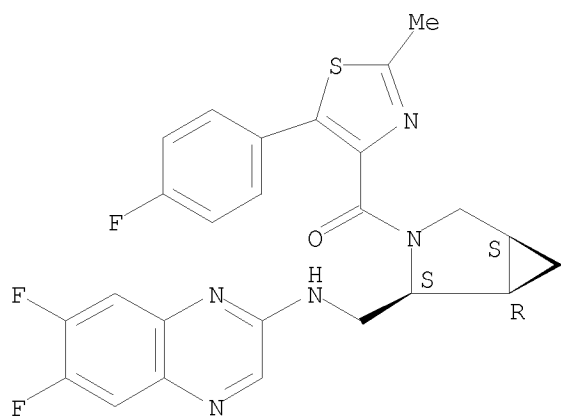
Relative stereochemistry.



RN 1017267-05-8 CAPLUS

CN Methanone, [(1R,2S,5S)-2-[[(6,7-difluoro-2-quinoxaliny)amino]methyl]-3-azabicyclo[3.1.0]hex-3-yl][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]-, rel- (CA INDEX NAME)

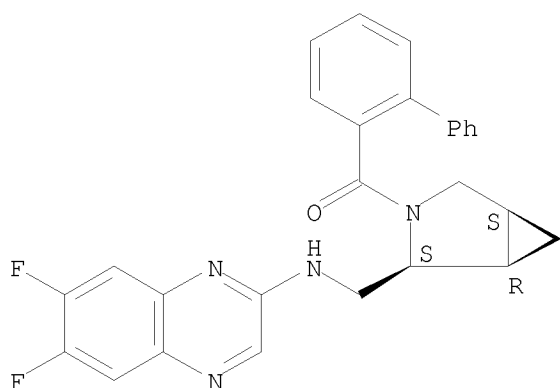
Relative stereochemistry.



RN 1017267-06-9 CAPLUS

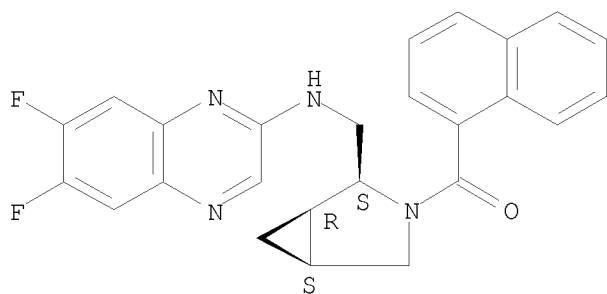
CN Methanone, [1,1'-biphenyl]-2-yl[(1R,2S,5S)-2-[[(6,7-difluoro-2-quinoxaliny)amino]methyl]-3-azabicyclo[3.1.0]hex-3-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



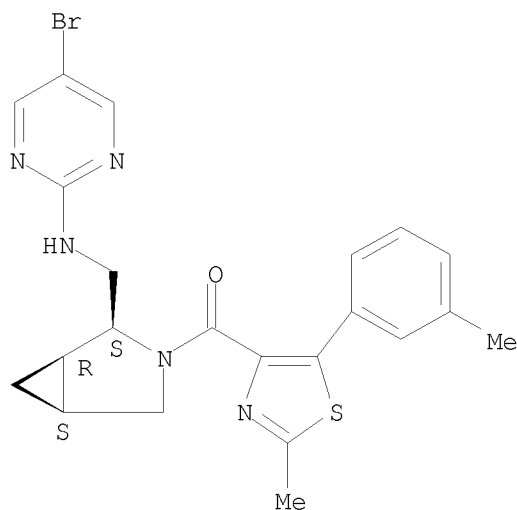
RN 1017267-07-0 CAPLUS
 CN Methanone, [(1R,2S,5S)-2-[[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-3-azabicyclo[3.1.0]hex-3-yl]-1-naphthalenyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



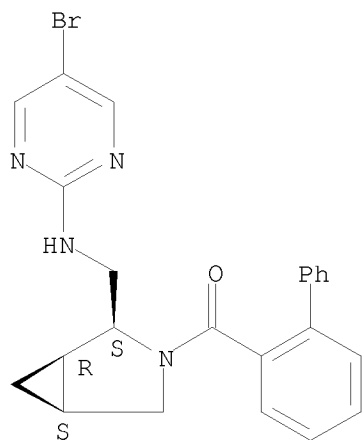
RN 1017267-08-1 CAPLUS
 CN Methanone, [(1R,2S,5S)-2-[[[5-bromo-2-pyrimidinyl]amino]methyl]-3-azabicyclo[3.1.0]hex-3-yl][2-methyl-5-(3-methylphenyl)-4-thiazolyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



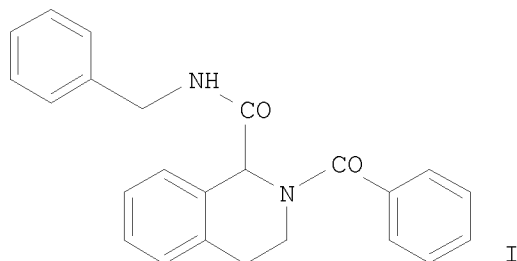
RN 1017267-09-2 CAPLUS
 CN Methanone, [1,1'-biphenyl]-2-yl[(1R,2S,5S)-2-[[5-bromo-2-pyrimidinyl]amino]methyl]-3-azabicyclo[3.1.0]hex-3-yl-, rel- (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:855521 CAPLUS
 DOCUMENT NUMBER: 147:406662
 TITLE: IBX-mediated oxidative Ugi-type multicomponent reactions: application to the N and C1 functionalization of tetrahydroisoquinoline
 AUTHOR(S): Ngouansavanh, Tifelle; Zhu, Jieping
 CORPORATE SOURCE: ICSN, CNRS, Gif-sur-Yvette Cedex, 91198, Fr.
 SOURCE: Angewandte Chemie, International Edition (2007), 46(30), 5775-5778
 CODEN: ACIEF5; ISSN: 1433-7851

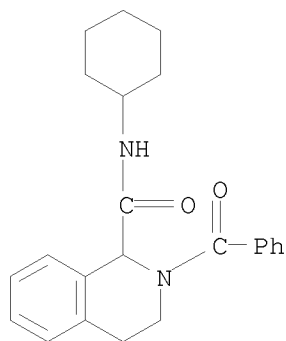
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 147:406662
 GI



AB An Ugi-type reaction of tetrahydroisoquinoline with an isocyanide and a carboxylic acid in the presence of iodoxybenzoic acid (IBX) afforded the 1,2-diacylated adduct in good to excellent yields. E.g., in the presence of IBX, reaction of 1,2,3,4-tetrahydroisoquinoline, PhCO₂H, and BnNC gave 87% 2-benzoyl-N-benzyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (I).

IT 950829-54-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (dual N and C1 acylation of tetrahydroisoquinoline by IBX-mediated oxidative Ugi-type multicomponent reactions with isocyanides and carboxylic acids)

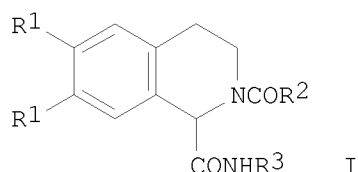
RN 950829-54-6 CAPLUS
 CN 1-Isoquinolinecarboxamide, 2-benzoyl-N-cyclohexyl-1,2,3,4-tetrahydro- (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:570695 CAPLUS
 DOCUMENT NUMBER: 148:100490
 TITLE: Synthesis of 1,2,3,4-tetrahydroisoquinoline-1-carboxylic acid derivatives via Ugi reactions
 AUTHOR(S): Schuster, Ildiko; Sztojkov-Ivanov, Anita; Lazar,

CORPORATE SOURCE: Laszlo; Fulop, Ferenc
Institute of Pharmaceutical Chemistry, University of Szeged, Szeged, H-6701, Hung.
SOURCE: Letters in Organic Chemistry (2007), 4(2), 102-108
CODEN: LOCEC7; ISSN: 1570-1786
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:100490
GI

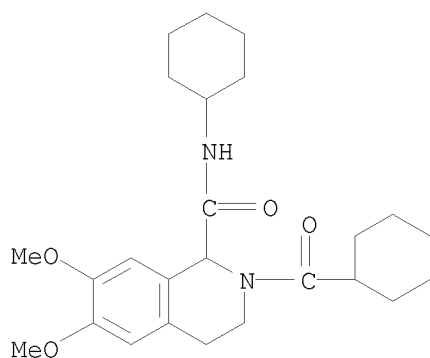


AB The three-component Ugi reactions of 3,4-dihydroisoquinolines, isocyanides and acids furnished 2-acyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamides (I; R1 = H, MeO; R2 = Ph, cyclohexyl; R3 = benzyl, cyclohexyl) in moderate to good yields. Chiral, nonracemic acids induced only poor diastereoselectivities in the condensations. Hydrolysis of the Ugi carboxamides gave 1,2,3,4-tetrahydroisoquinoline-1-carboxylic acids, which, due to their ready ability to undergo racemization, were obtained as racemic mixts. or with low enantiomeric excesses.

IT 1000368-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tetrahydroisoquinolinecarboxylic acids via Ugi multicomponent condensation of dihydroisoquinolines with carboxylic acids and isocyanides)

RN 1000368-67-1 CAPLUS

CN 1-Isoquinolinecarboxamide, N-cyclohexyl-2-(cyclohexylcarbonyl)-1,2,3,4-tetrahydro-6,7-dimethoxy- (CA INDEX NAME)

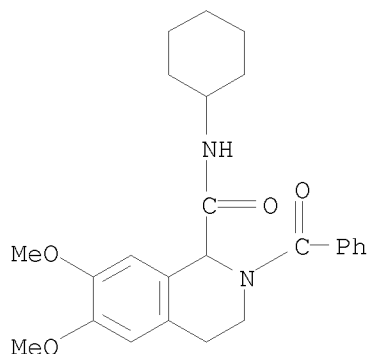


IT 1000368-66-0P
RL: SPN (Synthetic preparation); PREP (Preparation)

(tetrahydroisoquinolinecarboxylic acids via Ugi multicomponent condensation of dihydroisoquinolines with carboxylic acids and isocyanides)

RN 1000368-66-0 CAPLUS

CN 1-Isoquinolinecarboxamide, 2-benzoyl-N-cyclohexyl-1,2,3,4-tetrahydro-6,7-dimethoxy- (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:945697 CAPLUS

DOCUMENT NUMBER: 145:335949

TITLE: Preparation of tetrahydroisoquinoline compounds as ACAT inhibitors

INVENTOR(S): Takahashi, Kenji; Shirahase, Hiroaki; Kunishiro, Kazuhiro; Kasai, Masayasu

PATENT ASSIGNEE(S): Kyoto Pharmaceutical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 175pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

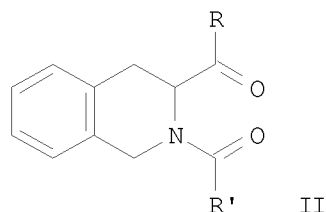
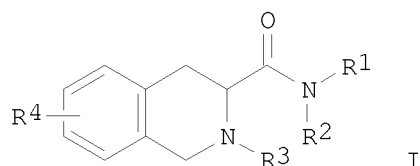
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006095922	A1	20060914	WO 2006-JP305301	20060310
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
EP 1857444	A1	20071121	EP 2006-729291	20060310

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
 PRIORITY APPLN. INFO.: JP 2005-67596 A 20050310
 WO 2006-JP305301 W 20060310
 OTHER SOURCE(S): MARPAT 145:335949
 GI

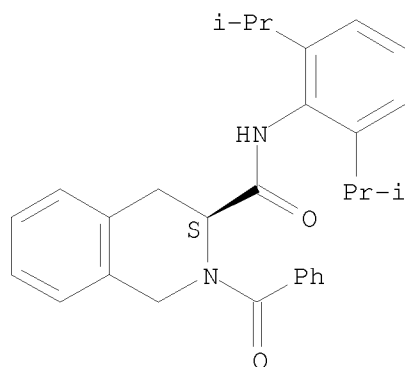


AB Title compds. I [R1, R2 = H, alkyl, cycloalkyl, etc.; R3 = (un)substituted alkyl, (un)substituted carbamoyl, (un)substituted aminosulfonyl, etc.; R4 = H, hydroxy, (un)substituted alkoxy, etc.] and their pharmaceutically acceptable salts were prepared For example, reaction of 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid hydrochloride with 2,6-diisopropylphenylisocyanate followed by EDCI mediated amidation with piperidine afforded compound II [R = piperidin-1-yl; R' = 2,6-diisopropylphenylamino]. In acyl-CoA:cholesterolacyltransferase (ACAT) inhibition assays, compound (3S)-II [R = 2,6-diisopropylphenylamino; R' = n-heptyl] exhibited the activity of 93.3% at 10⁻⁶ M. Compds. I are claimed useful for the treatment of hyperlipidemia, arteriosclerosis, etc.

IT 909570-94-1P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of tetrahydroisoquinoline compds. as ACAT inhibitors for treatment of hyperlipidemia and arteriosclerosis)

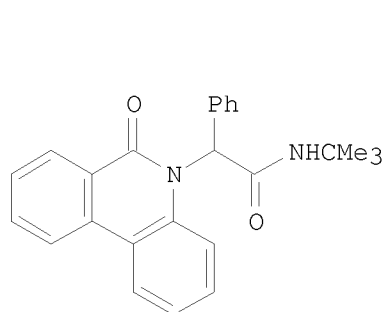
RN 909570-94-1 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-benzoyl-N-[2,6-bis(1-methylethyl)phenyl]-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.

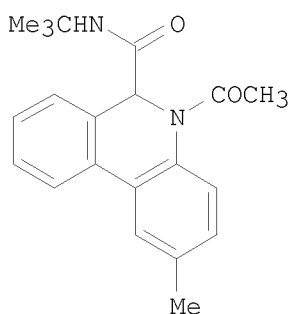


REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:729423 CAPLUS
 DOCUMENT NUMBER: 145:335963
 TITLE: Synthesis of Functionalized Quinolines via Ugi and Pd-Catalyzed Intramolecular Arylation Reactions
 AUTHOR(S): Ma, Zhibo; Xiang, Zheng; Luo, Tuoping; Lu, Kui; Xu, Zhibin; Chen, Jiahua; Yang, Zhen
 CORPORATE SOURCE: Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education and Beijing National Laboratory for Molecular Science (BNLMS), College of Chemistry, the State Key Laboratory of Natural and Biomimetic Drugs, School of Pharmaceutical Science, Laboratory of Chemical Genomics, Shenzhen Graduate School Peking University, Beijing, 100871, Peop. Rep. China
 SOURCE: Journal of Combinatorial Chemistry (2006), 8(5), 696-704
 CODEN: JCCHFF; ISSN: 1520-4766
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:335963
 GI



I



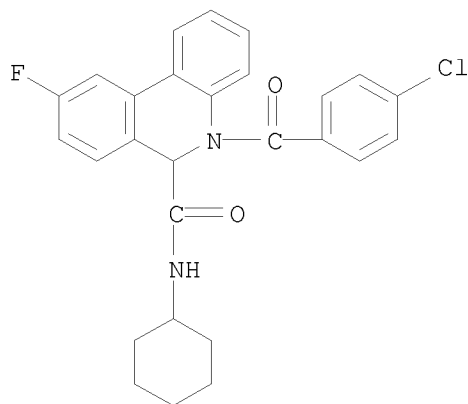
II

AB Two types of quinoline scaffolds were constructed in a combinatorial format via the Ugi four-component reaction and Pd-catalyzed intramol. arylation reaction. For example, Ugi reaction of 2-iodobenzoic acid, aniline, benzaldehyde and tert-Bu isonitrile gave the intermediate bis-amide, which underwent intramol. arylation reaction to give phenanthridinone I. On the other hand, multicomponent reaction of p-toluidine, 2-iodobenzaldehyde, acetic acid and tert-Bu isonitrile followed by Pd-catalyzed intramol. arylation gave (carbamoyl)dihydrophenanthridine II. Several quinolinone-fused benzofurans, benzothiophenes and indoles were similarly prepared. The scope of this two-step synthetic sequence was examined from com. available and synthetically accessible starting materials.

IT 909545-57-9P 909545-58-0P 909545-60-4P 909545-61-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of functionalized phenanthridines and heterocycle-fused quinolines via four-component Ugi condensation of aromatic aldehydes, anilines, isonitriles and carboxylic acids followed by Pd-catalyzed intramol. arylation reactions)

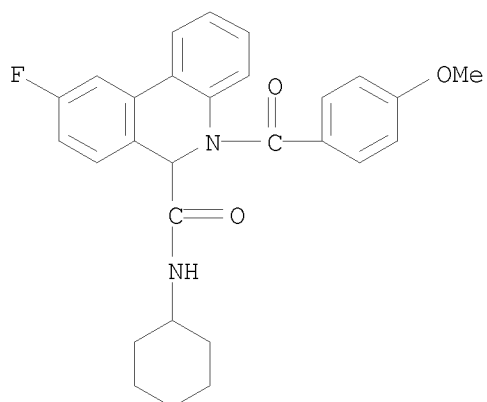
RN 909545-57-9 CAPLUS

CN 6-Phenanthridinecarboxamide, 5-(4-chlorobenzoyl)-N-cyclohexyl-9-fluoro-5,6-dihydro- (CA INDEX NAME)



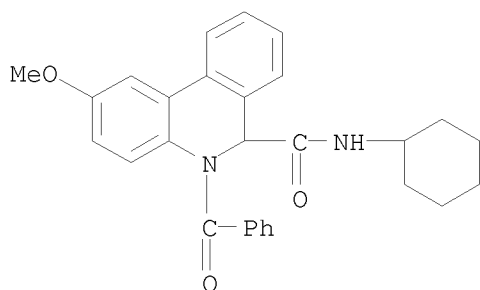
RN 909545-58-0 CAPLUS

CN 6-Phenanthridinecarboxamide, N-cyclohexyl-9-fluoro-5,6-dihydro-5-(4-methoxybenzoyl)- (CA INDEX NAME)



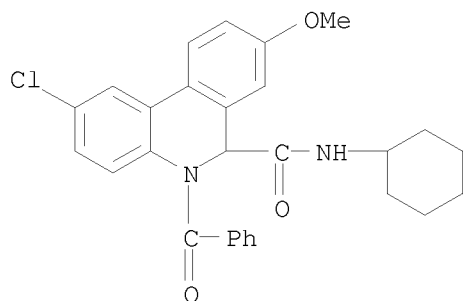
RN 909545-60-4 CAPLUS

CN 6-Phenanthridinecarboxamide, 5-benzoyl-N-cyclohexyl-5,6-dihydro-2-methoxy-
(CA INDEX NAME)



RN 909545-61-5 CAPLUS

CN 6-Phenanthridinecarboxamide, 5-benzoyl-2-chloro-N-cyclohexyl-5,6-dihydro-8-methoxy-
(CA INDEX NAME)



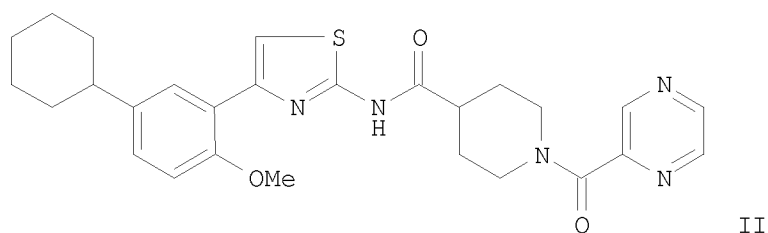
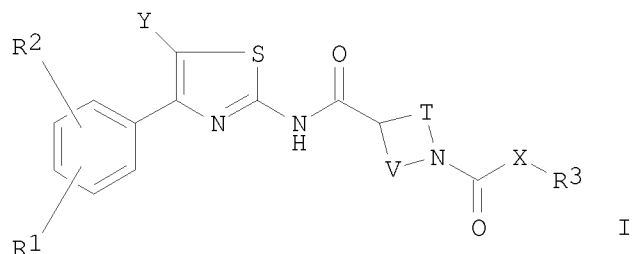
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:365129 CAPLUS

DOCUMENT NUMBER: 144:412491
 TITLE: Preparation of 2-amido-4-phenylthiazole derivatives as chemokine receptors modulators, in particular MCP-1 and CCR2b receptor antagonists, and their therapeutic application
 INVENTOR(S): Casellas, Pierre; Floutard, Daniel; Fraisse, Pierre; Jegham, Samir
 PATENT ASSIGNEE(S): Sanofi Aventis, Fr.
 SOURCE: Fr. Demande, 94 pp.
 CODEN: FRXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2876692	A1	20060421	FR 2004-11083	20041019
FR 2876692	B1	20070223		
AU 2005296958	A1	20060427	AU 2005-296958	20051017
CA 2584774	A1	20060427	CA 2005-2584774	20051017
WO 2006042954	A1	20060427	WO 2005-FR2565	20051017
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
EP 1807421	A1	20070718	EP 2005-809089	20051017
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU			
CN 101065376	A	20071031	CN 2005-80039696	20051017
JP 2008517042	T	20080522	JP 2007-537324	20051017
US 20070259847	A1	20071108	US 2007-736770	20070418
MX 200704740	A	20070618	MX 2007-4740	20070419
IN 2007KN01611	A	20070727	IN 2007-KN1611	20070504
NO 2007002515	A	20070628	NO 2007-2515	20070516
KR 2007085395	A	20070827	KR 2007-711308	20070518
PRIORITY APPLN. INFO.:			FR 2004-11083	A 20041019
			WO 2005-FR2565	W 20051017
OTHER SOURCE(S):			CASREACT 144:412491; MARPAT 144:412491	
GI				



AB Title compds. I [R1 = H, halo, alkyl, allyloxy, etc.; R2 = H, halo, OH and derivs., perfluoroalkyl, etc.; Y = H, halo; R3 = (un)substituted Ph, heterocyclyl, heterobicyclyl; T = (CH2)m; m = 2-4; V = (CH2)n; n = 0-2; X = (CH2)p; p = 0-3; their free bases, acid addition salts, and their hydrates and solvates, and their enantiomers, diastereomers, and mixts.] were prepared as chemokine receptors modulators, in particular Monocyte chemoattractant protein-1 (MCP-1) receptor and CC chemokine receptor (CCR2b) antagonists. Thus, reacting N-(tert-butoxycarbonyl)isonipetric acid with 4-(5-cyclohexylphenyl-2-methoxy)-1,3-thiazol-2-amine (preparation given), followed by Boc-deprotection and acylation with 1-pyrazinecarboxylic acid gave phenylthiazole II (m.p. = 129°). I displayed IC50 values < 1 μM for chemotaxis inhibition towards hMCP-1 and CCR2b, demonstrating their antagonistic activity towards chemokine receptors. Thus, I are useful for treating immuno-inflammatory syndromes, allergies, and angiogenesis-mediated diseases, bacterial and viral infections, cardiac diseases, and obesity.

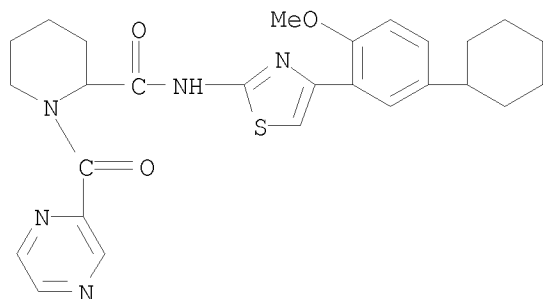
IT 884326-78-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of 2-amido-4-phenylthiazoles as chemokine receptor MCP-1 and CCR2b modulators, especially antagonists, and their therapeutic application)

RN 884326-78-7 CAPLUS

CN 2-Piperidinecarboxamide, N-[4-(5-cyclohexyl-2-methoxyphenyl)-2-thiazolyl]-1-(2-pyrazinylcarbonyl)- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:735326 CAPLUS

DOCUMENT NUMBER: 143:229730

TITLE: Preparation of tetrahydroisoquinoline derivatives for treating diseases mediated by protein trafficking or chloride channel activity

INVENTOR(S): Pregel, Marko J.; Hirth, Bradford H.; Kane, John L.; Qiao, Shuang; Gregory, Jill; Cuff, Lisa

PATENT ASSIGNEE(S): Genzyme Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 52 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

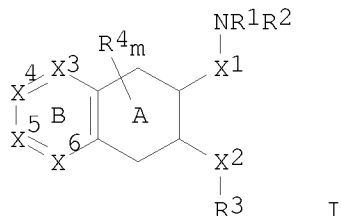
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050176761	A1	20050811	US 2004-6042	20041207
PRIORITY APPLN. INFO.:			US 2003-531873P	P 20031223
OTHER SOURCE(S):			CASREACT 143:229730; MARPAT 143:229730	

GI



AB Tetrahydroisoquinoline derivs. I (variables defined below), pharmaceutical compns. comprising them and methods of treating disease are disclosed herein. The disclosed compds. are useful in the treatment and prevention of diseases mediated by chloride channel activity and/or protein trafficking, including, but not limited to, diseases associated with impaired

mucociliary clearance such as cystic fibrosis, bronchitis, emphysema, and the like. For I the variables are: X1 = CH2, CO, SO, SO2; X2 = CH2, CO, COCH2, CO2, COS, O, S, SO; X3, X4, X5, X6 = N, CH, wherein at least 1 of X3, X4, X5, X6 = CH; Ring B is optionally substituted in any substitutable carbon; R1 and R2 = H or an optionally substituted aliphatic, aryl, heteroaryl, heterocyclic, cycloalkyl, peptide, or amino acid group, provided that R1 and R2 are not both H; or, R1 and R2, taken together with the nitrogen to which they are bonded, are an optionally substituted heterocyclic group; R3 = optionally substituted aryl, heteroaryl, cycloalkyl, or heterocyclic group; m = 0-2; each R4 = halogen, OH, SH, Ra, ORa, SRa, NH2, NHRa, NRa2, C(O)NRa2, CF3, CN, or NO2; and Ra = C1-C5 branched or linear alkyl group.

IT 851777-43-0P 851777-46-3P 851777-47-4P
 851777-48-5P 851777-49-6P 851777-50-9P
 851777-52-1P 851777-53-2P 851777-54-3P,
 2-(3-Phenoxybenzoyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid
 N-(4-heptylphenyl)amide 851777-55-4P 851777-56-5P
 851777-57-6P 851777-59-8P 851777-60-1P
 851777-61-2P 851777-62-3P 851777-63-4P,
 (S)-2-(3-Phenoxybenzoyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid
 N-(6-pentylpyridin-3-yl)amide 851777-64-5P 851777-66-7P
 851777-67-8P 851777-68-9P 851777-69-0P
 851777-71-4P 851777-73-6P 851777-76-9P
 851777-77-0P 851777-79-2P 851777-80-5P
 851777-81-6P 851777-83-8P 851777-84-9P
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 851777-93-0P, (S)-2-[[5-(Cyclohexyloxy)pyridin-3-yl]carbonyl]-
 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid N-(4-pentylphenyl)amide
 851777-94-1P 851777-95-2P, (S)-2-(2-Isopropoxypyridine-4-
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 (4-pentylphenyl)amide 862504-12-9P 862504-13-0P
 862504-14-1P 862504-15-2P 862504-16-3P
 862504-17-4P 862504-18-5P 862504-19-6P
 862504-20-9P 862504-21-0P 862504-22-1P
 862504-23-2P 862504-24-3P, 2-[(Naphthalen-2-yl)carbonyl]-
 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid N-(4-chlorophenyl)amide
 862504-25-4P 862504-26-5P 862504-27-6P
 862504-31-2P 862504-32-3P 862504-36-7P
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 862504-90-3P 862504-93-6P 862505-04-2P
 862505-09-7P 862505-12-2P 862505-21-3P,
 2-(3-Phenoxybenzoyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid
 N-[4-[(acetyl)(hexyl)amino]phenyl]amide 862505-24-6P
 862505-33-7P, 2-(3-Phenoxybenzoyl)-1,2,3,4-tetrahydroisoquinoline-
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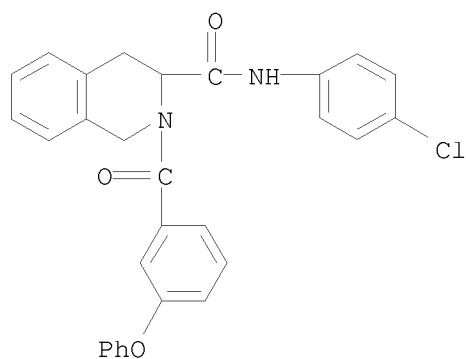
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 862505-68-8P 862505-71-3P 862505-74-6P
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 862505-96-2P, (S)-2-[4-Ethoxy-3-phenoxy-benzoyl]-1,2,3,4-
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 862506-01-2P 862506-10-3P 862506-13-6P,
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 tetrahydroisoquinoline-3-carboxylic acid N-(4-pentylphenyl)amide
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 862506-34-1P 862506-36-3P 862506-38-5P
 862506-41-0P 862506-44-3P 862506-47-6P
 862506-52-3P 862506-57-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(drug candidate; preparation of tetrahydroisoquinoline derivs. for treating
 diseases mediated by protein trafficking or chloride channel activity)

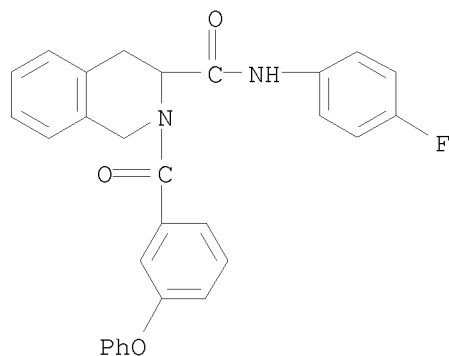
RN 851777-43-0 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(3-
 phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-46-3 CAPLUS

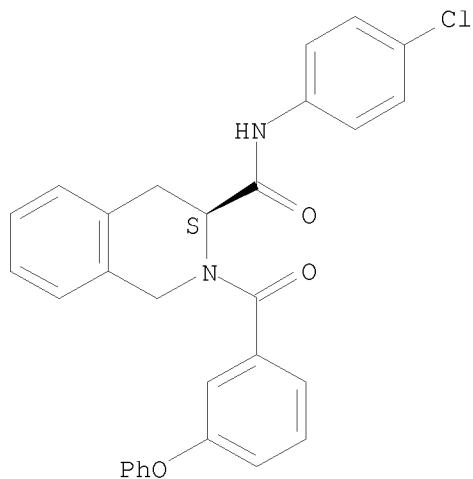
CN 3-Isoquinolinecarboxamide, N-(4-fluorophenyl)-1,2,3,4-tetrahydro-2-(3-
 phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-47-4 CAPLUS

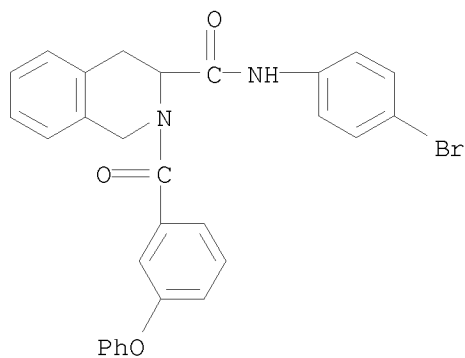
CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



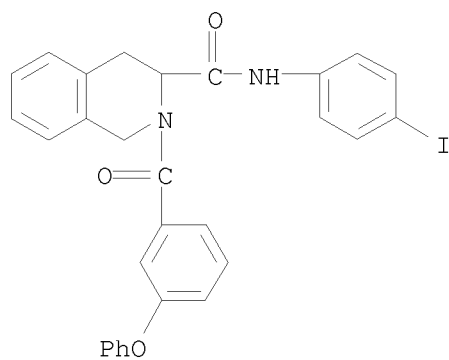
RN 851777-48-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-bromophenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



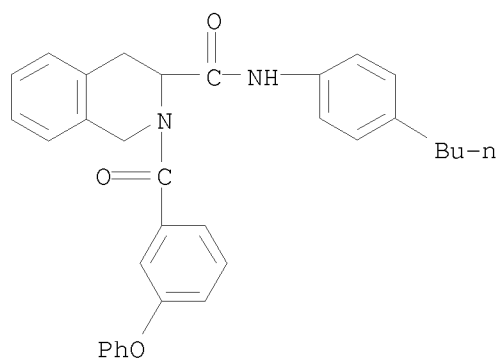
RN 851777-49-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-iodophenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-50-9 CAPLUS

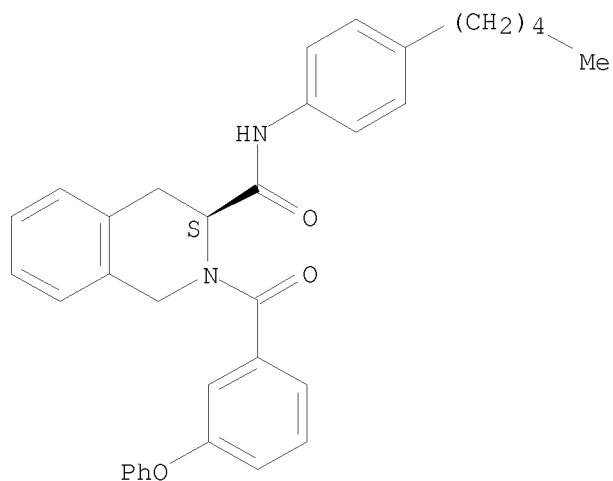
CN 3-Isoquinolinecarboxamide, N-(4-butylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-52-1 CAPLUS

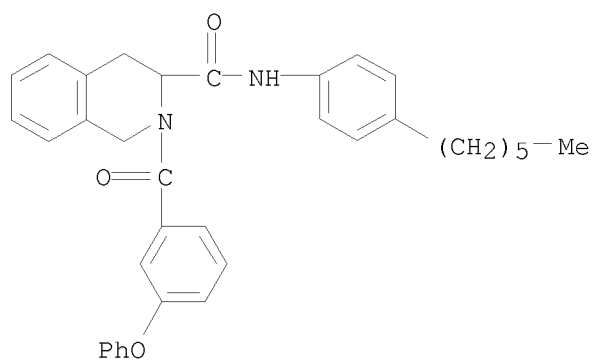
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



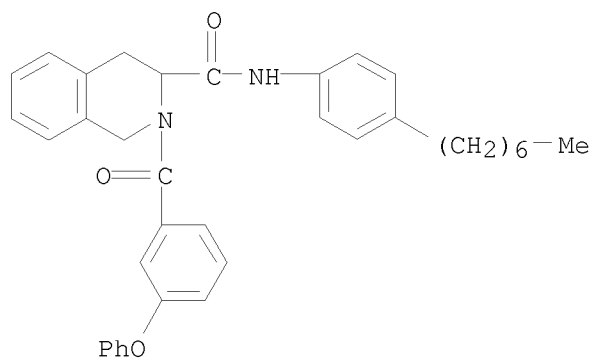
RN 851777-53-2 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-hexylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



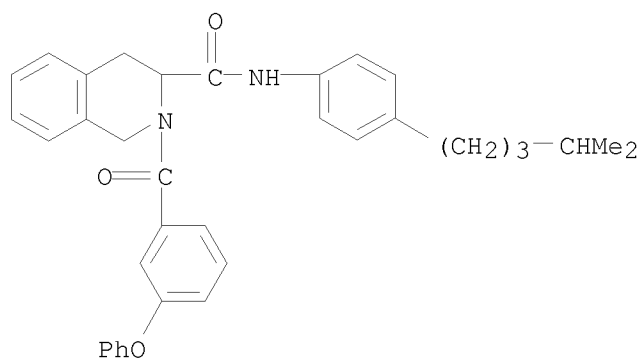
RN 851777-54-3 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-heptylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



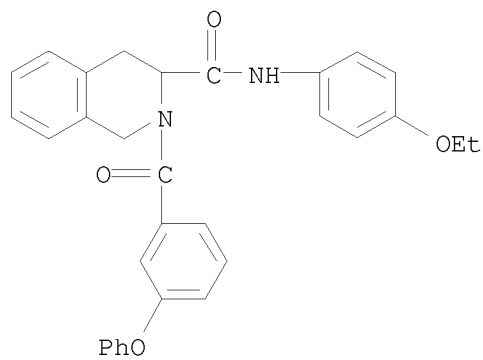
RN 851777-55-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[4-(4-methylpentyl)phenyl]-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



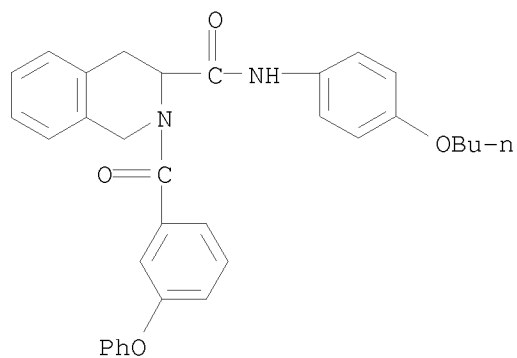
RN 851777-56-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-ethoxyphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



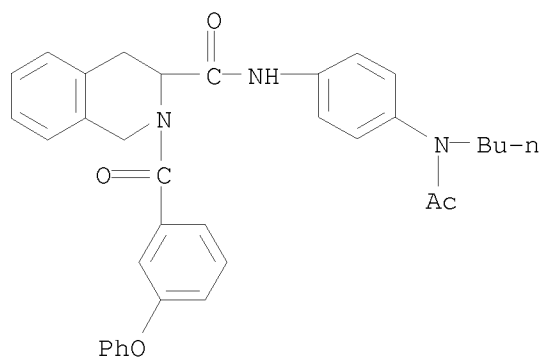
RN 851777-57-6 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-butoxyphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



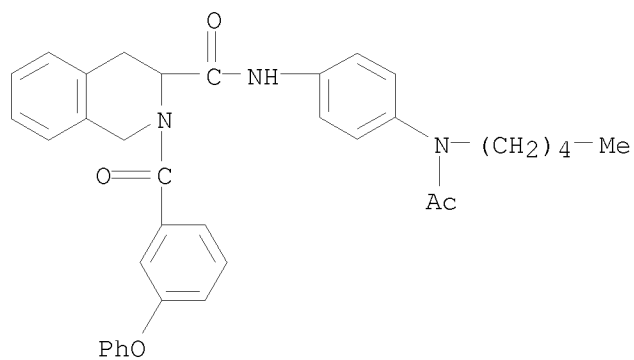
RN 851777-59-8 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-(acetylbutylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



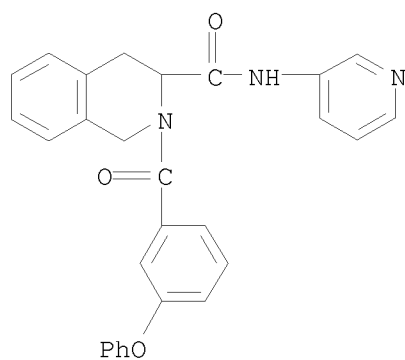
RN 851777-60-1 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-(acetylpentylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



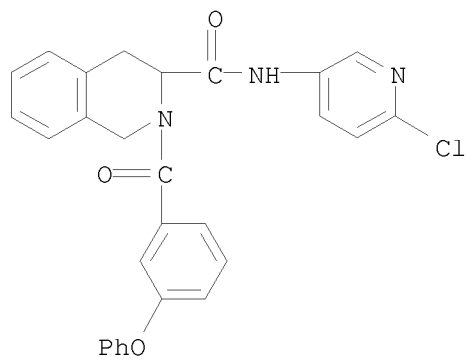
RN 851777-61-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-3-pyridinyl- (CA INDEX NAME)



RN 851777-62-3 CAPLUS

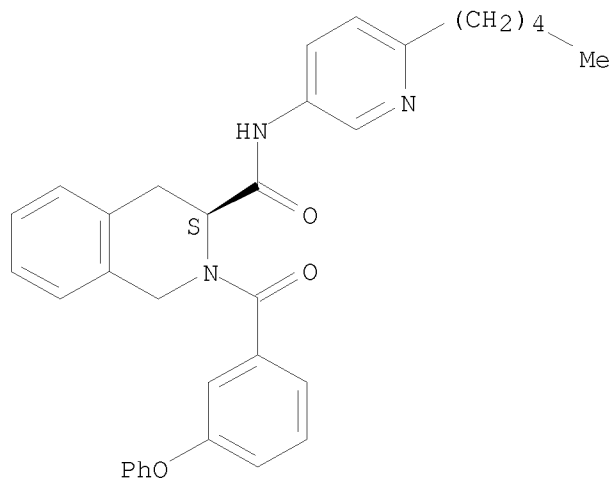
CN 3-Isoquinolinecarboxamide, N-(6-chloro-3-pyridinyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-63-4 CAPLUS

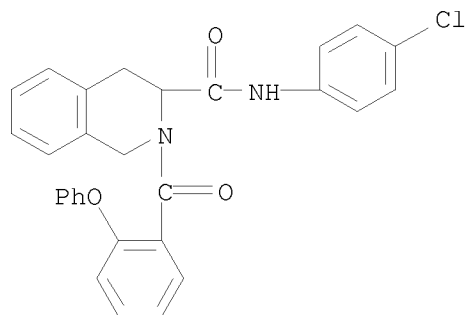
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(6-pentyl-3-pyridinyl)-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



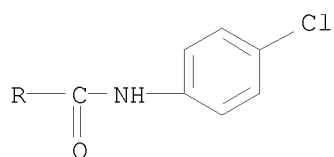
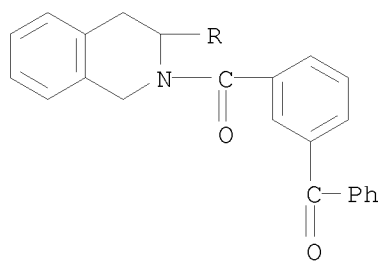
RN 851777-64-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(2-phenoxybenzoyl)- (CA INDEX NAME)

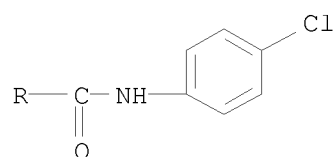
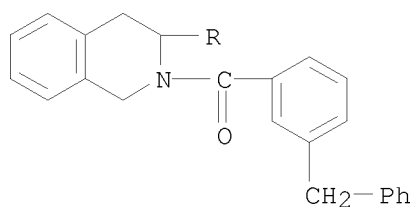


RN 851777-66-7 CAPLUS

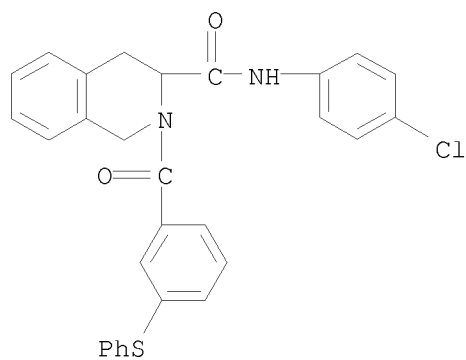
CN 3-Isoquinolinecarboxamide, 2-(3-benzoylbenzoyl)-N-(4-chlorophenyl)-1,2,3,4-tetrahydro- (CA INDEX NAME)



RN 851777-67-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(phenylmethyl)benzoyl]- (CA INDEX NAME)

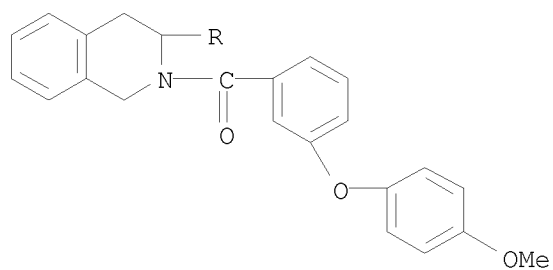


RN 851777-68-9 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(phenylthio)benzoyl]- (CA INDEX NAME)



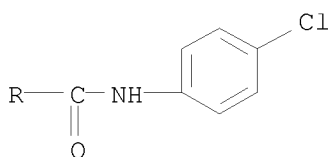
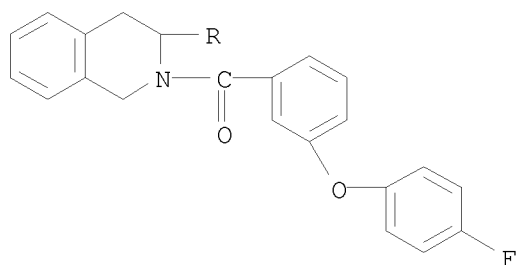
RN 851777-69-0 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(4-methoxyphenoxy)benzoyl]- (CA INDEX NAME)

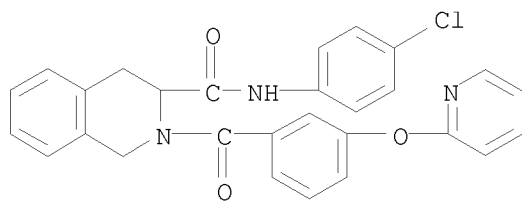


RN 851777-71-4 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-2-[3-(4-fluorophenoxy)benzoyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)

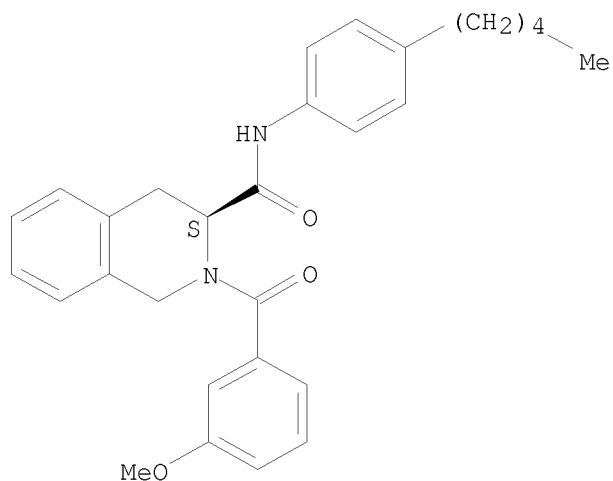


RN 851777-73-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(2-pyridinyloxy)benzoyl]- (CA INDEX NAME)



RN 851777-76-9 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-methoxybenzoyl)-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

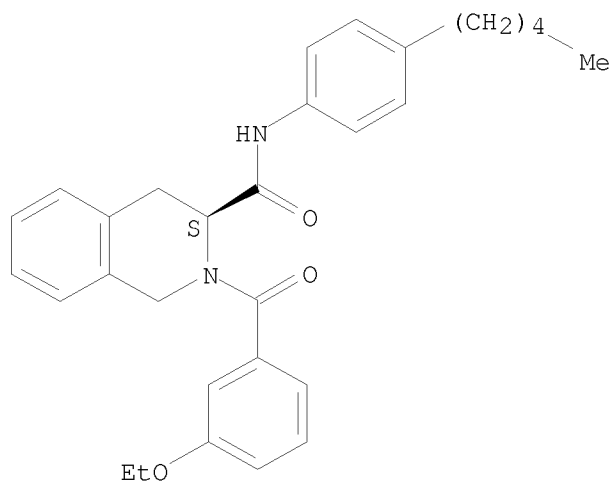
Absolute stereochemistry.



RN 851777-77-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-ethoxybenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

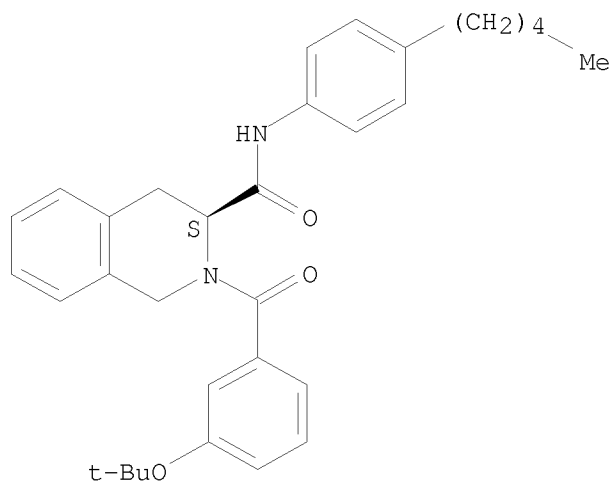
Absolute stereochemistry.



RN 851777-79-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(1,1-dimethylethoxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

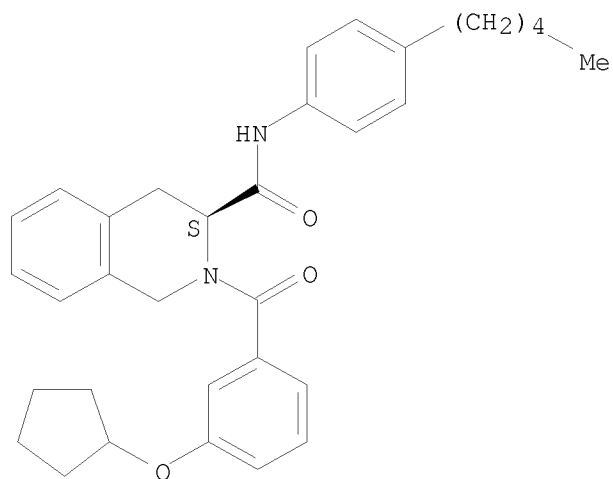
Absolute stereochemistry.



RN 851777-80-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(cyclopentyloxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

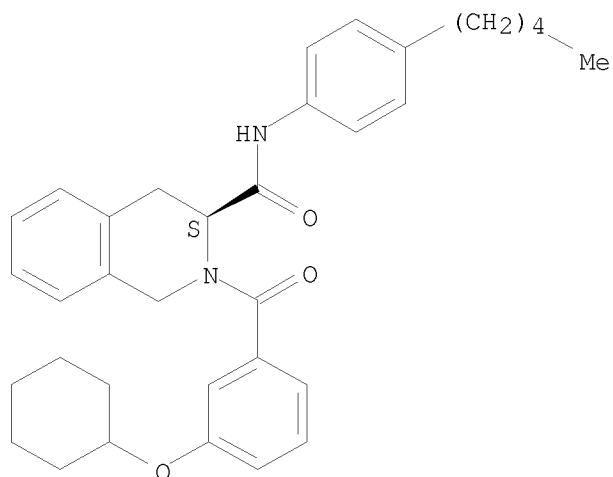
Absolute stereochemistry.



RN 851777-81-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(cyclohexyloxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

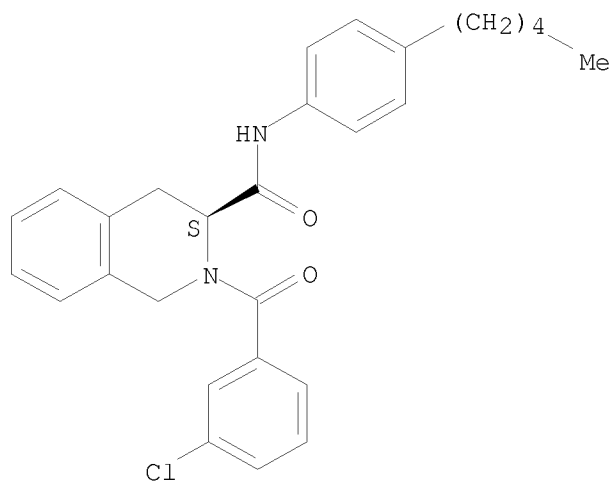
Absolute stereochemistry.



RN 851777-83-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-chlorobenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

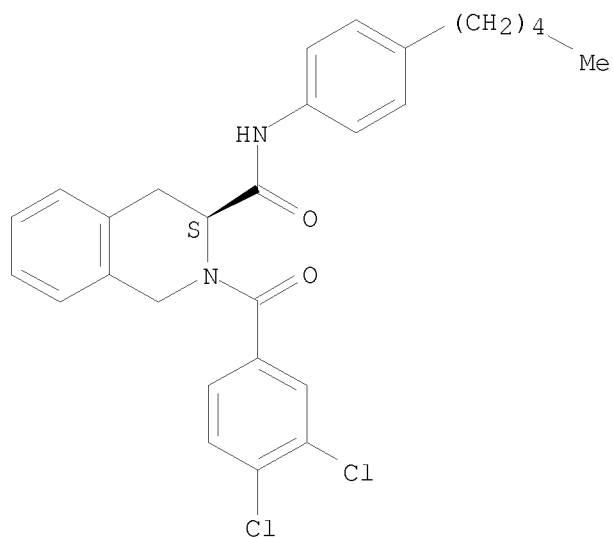
Absolute stereochemistry.



RN 851777-84-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3,4-dichlorobenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

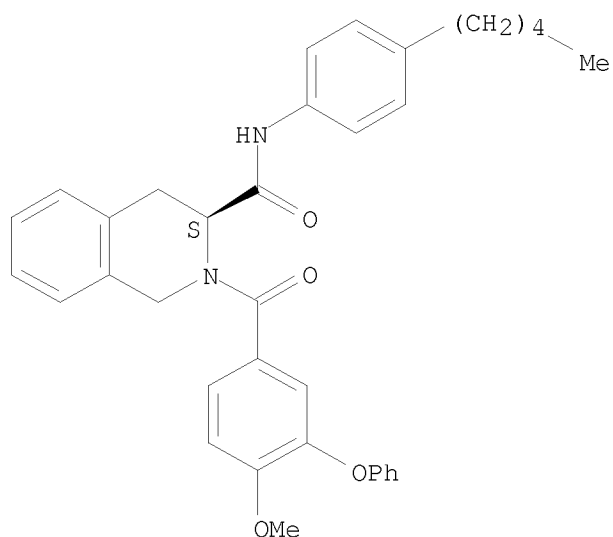
Absolute stereochemistry.



RN 851777-85-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methoxy-3-phenoxycarbonyl)-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

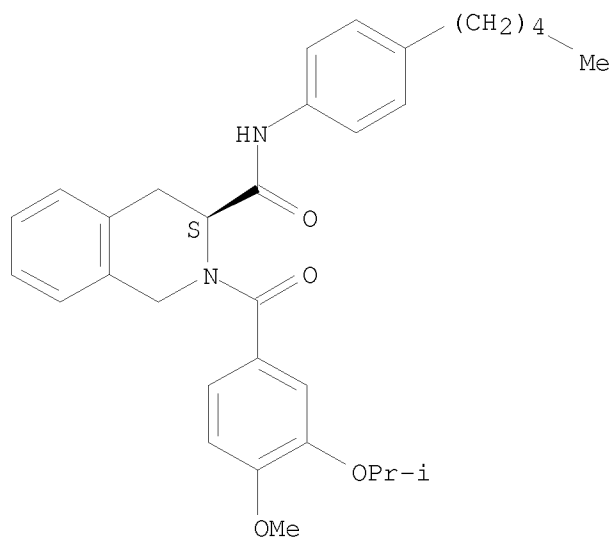
Absolute stereochemistry.



RN 851777-86-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[4-methoxy-3-(1-methylethoxy)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

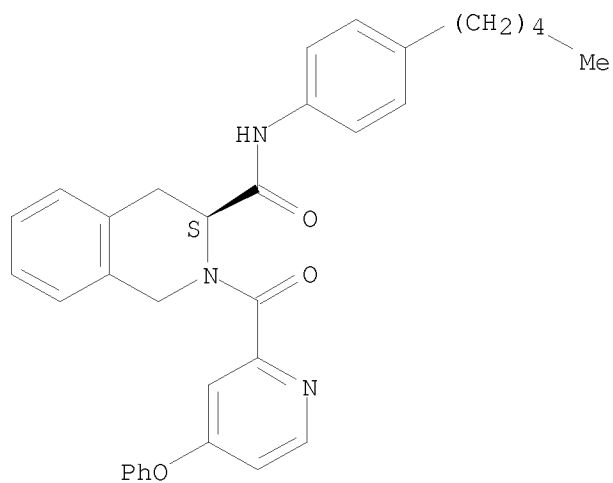
Absolute stereochemistry.



RN 851777-89-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-[(4-phenoxy-2-pyridinyl)carbonyl]-, (3S)- (CA INDEX NAME)

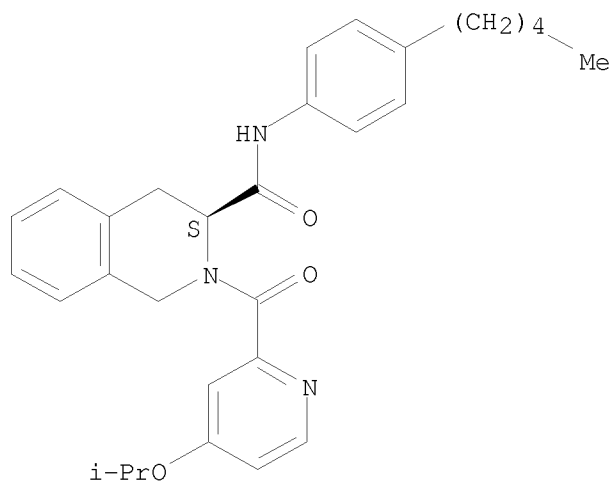
Absolute stereochemistry.



RN 851777-90-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[4-(1-methylethoxy)-2-pyridinyl]carbonyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

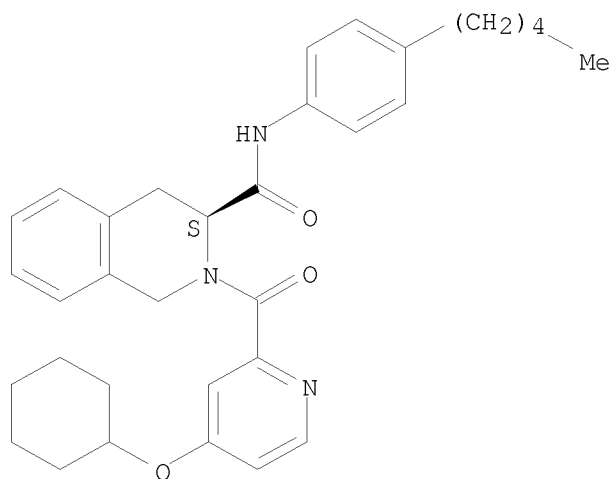
Absolute stereochemistry.



RN 851777-91-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[[4-(cyclohexyloxy)-2-pyridinyl]carbonyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

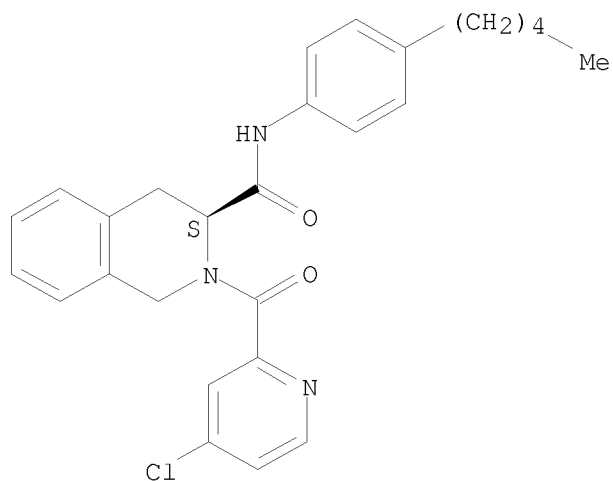
Absolute stereochemistry.



RN 851777-92-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[(4-chloro-2-pyridinyl)carbonyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

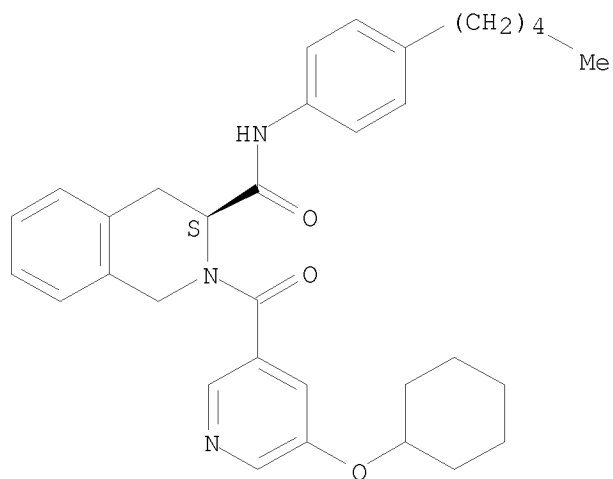
Absolute stereochemistry.



RN 851777-93-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[[5-(cyclohexyloxy)-3-pyridinyl]carbonyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

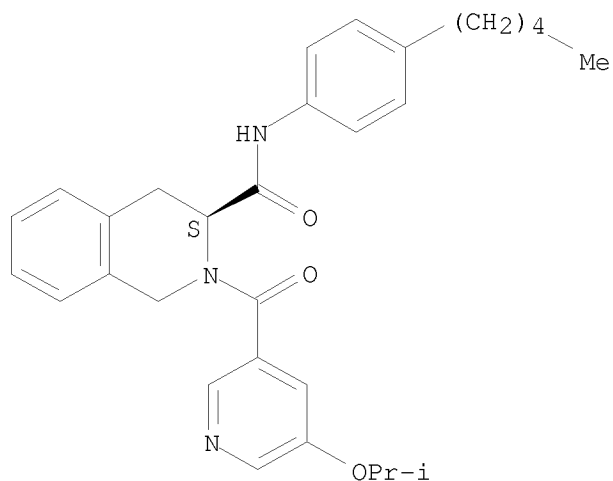
Absolute stereochemistry.



RN 851777-94-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[5-(1-methylethoxy)-3-pyridinyl]carbonyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

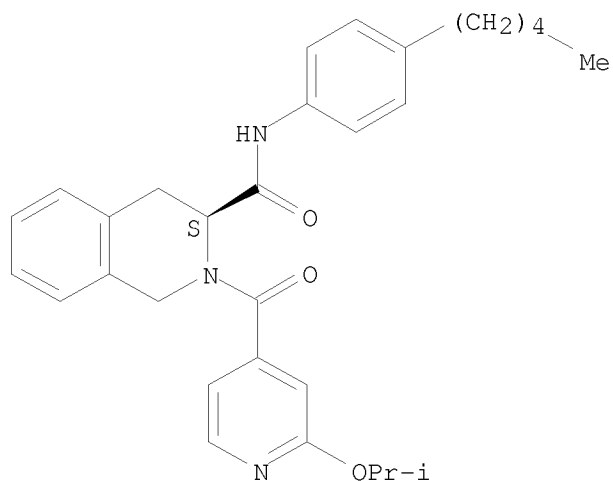
Absolute stereochemistry.



RN 851777-95-2 CAPLUS

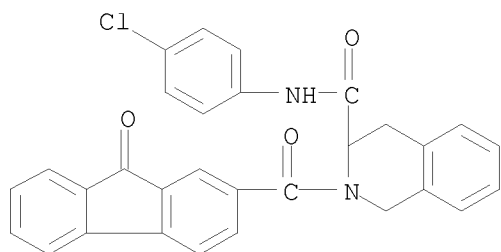
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[2-(1-methylethoxy)-4-pyridinyl]carbonyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



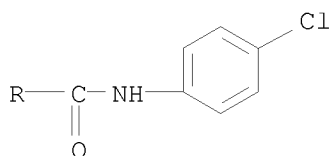
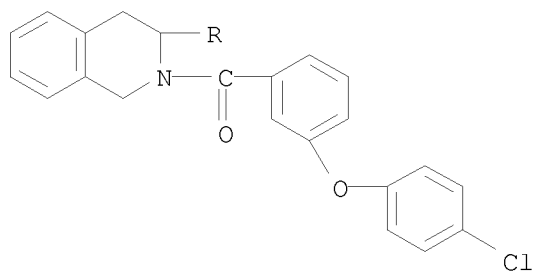
RN 862504-12-9 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[(9-oxo-9H-fluoren-2-yl)carbonyl]- (CA INDEX NAME)



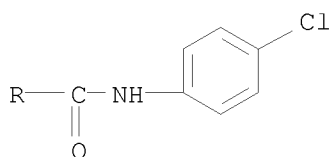
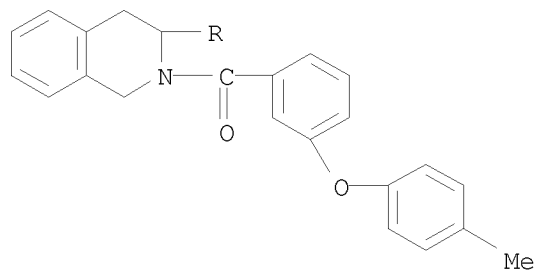
RN 862504-13-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(4-chlorophenoxy)benzoyl]-N-(4-chlorophenyl)-1,2,3,4-tetrahydro- (CA INDEX NAME)

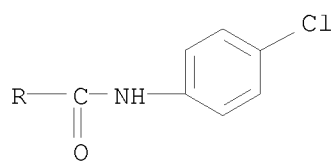
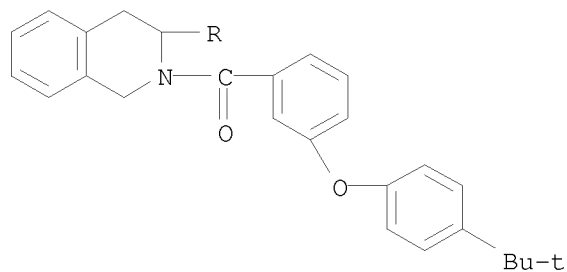


RN 862504-14-1 CAPLUS

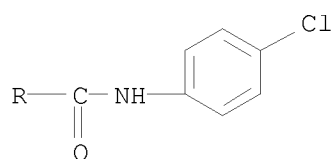
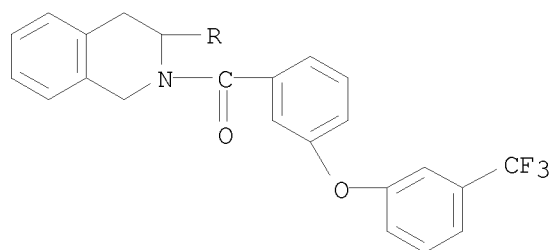
CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(4-methylphenoxy)benzoyl]- (CA INDEX NAME)



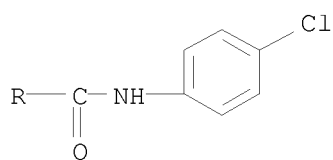
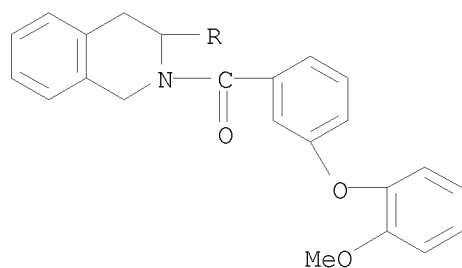
RN 862504-15-2 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-2-[3-[4-(1,1-dimethylethyl)phenoxy]benzoyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



RN 862504-16-3 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-[3-(trifluoromethyl)phenoxy]benzoyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)

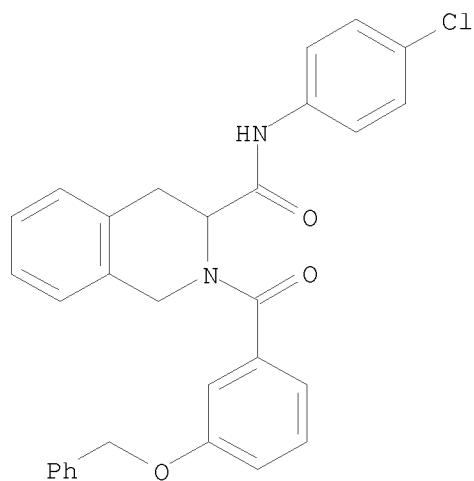


RN 862504-17-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(2-methoxyphenoxy)benzoyl]- (CA INDEX NAME)



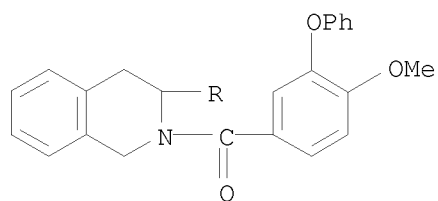
RN 862504-18-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(phenylmethoxy)benzoyl]-, (+)- (CA INDEX NAME)

Rotation (+).



RN 862504-19-6 CAPLUS

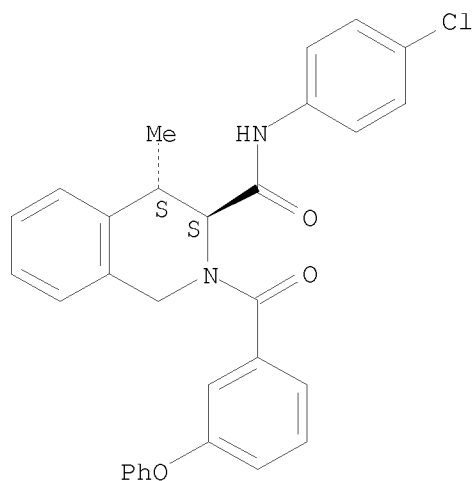
CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(4-methoxy-3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862504-20-9 CAPLUS

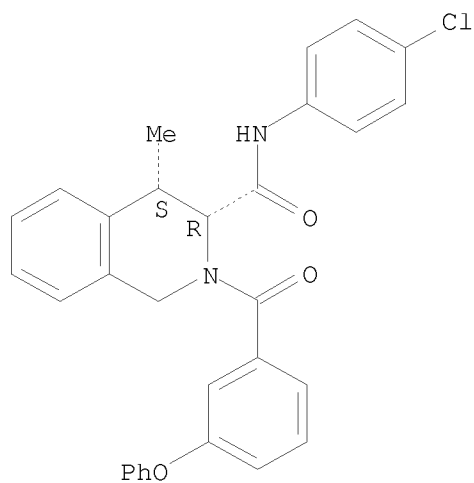
CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-4-methyl-2-(3-phenoxybenzoyl)-, (3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

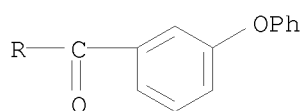
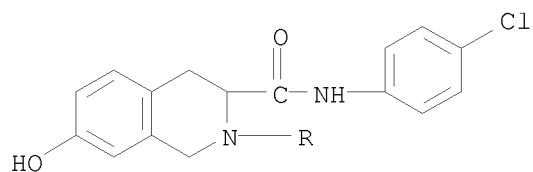


RN 862504-21-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-4-methyl-2-(3-phenoxybenzoyl)-, (3R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

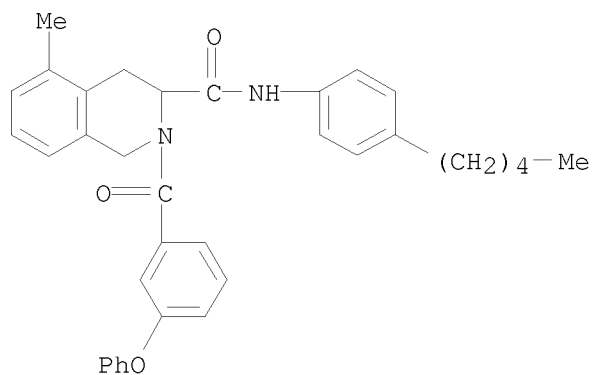


RN 862504-22-1 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-7-hydroxy-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



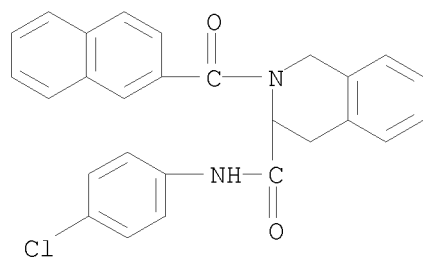
RN 862504-23-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-5-methyl-N-(4-pentylphenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



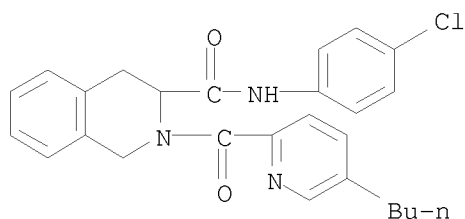
RN 862504-24-3 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(2-naphthalenylcarbonyl)- (CA INDEX NAME)



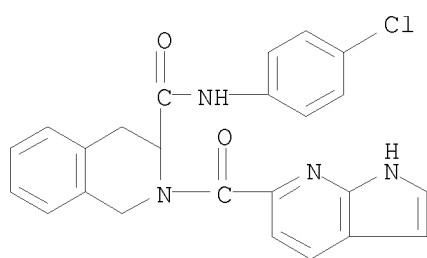
RN 862504-25-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[(5-butyl-2-pyridinyl)carbonyl]-N-(4-chlorophenyl)-1,2,3,4-tetrahydro- (CA INDEX NAME)



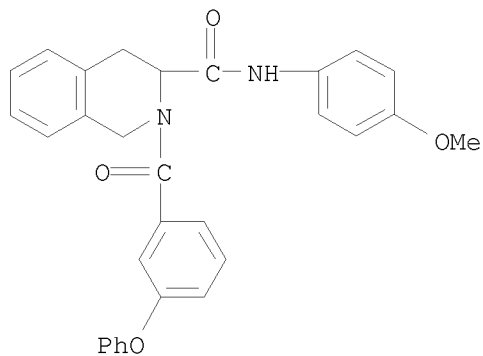
RN 862504-26-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(1H-pyrrolo[2,3-b]pyridin-6-ylcarbonyl)- (CA INDEX NAME)



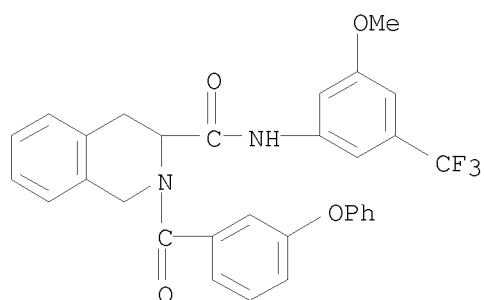
RN 862504-27-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-methoxyphenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



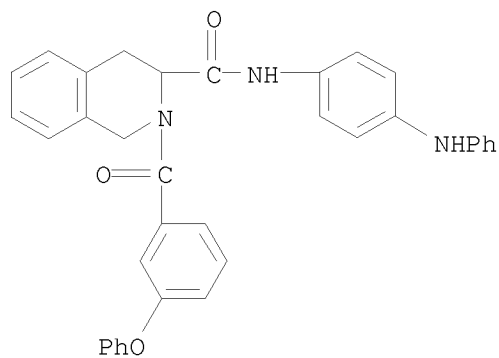
RN 862504-31-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[3-methoxy-5-(trifluoromethyl)phenyl]-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



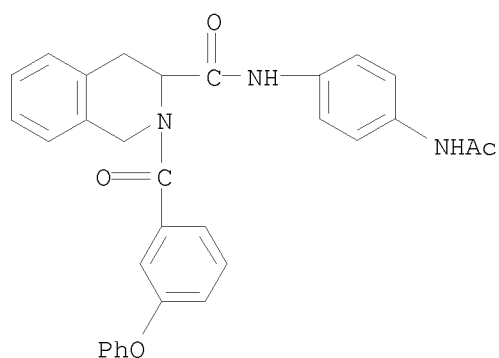
RN 862504-32-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-[4-(phenylamino)phenyl]- (CA INDEX NAME)



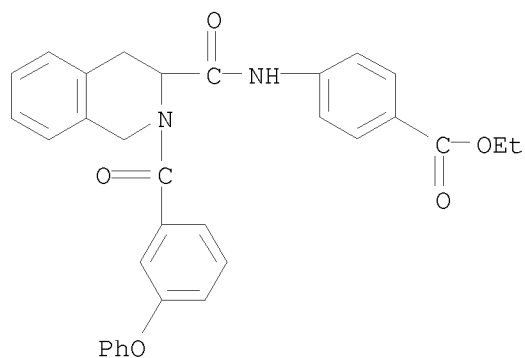
RN 862504-36-7 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-(acetylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



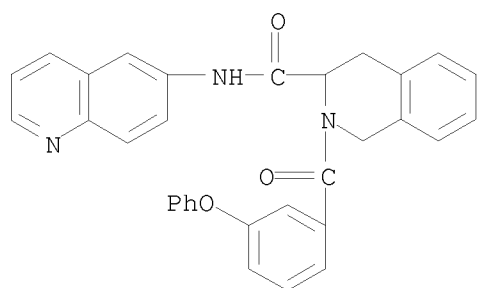
RN 862504-40-3 CAPLUS

CN Benzoic acid, 4-[[[1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-3-isoquinolinyl]carbonyl]amino]-, ethyl ester (CA INDEX NAME)



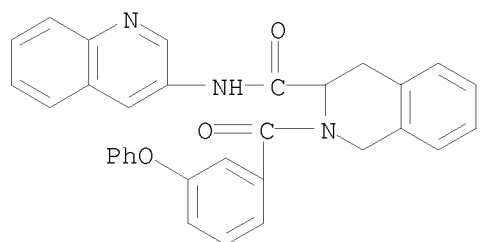
RN 862504-41-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-6-quinolinyl- (CA INDEX NAME)



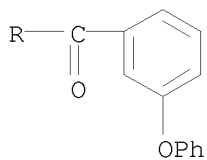
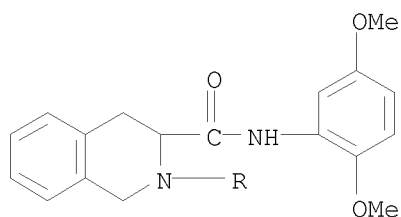
RN 862504-42-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-3-quinolinyl- (CA INDEX NAME)



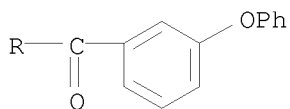
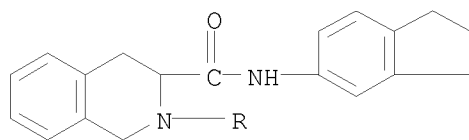
RN 862504-43-6 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(2,5-dimethoxyphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



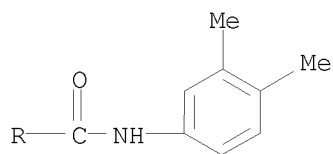
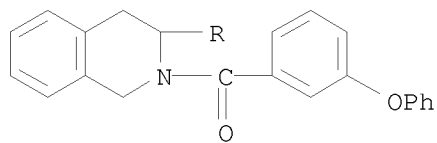
RN 862504-44-7 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(2,3-dihydro-1H-inden-5-yl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



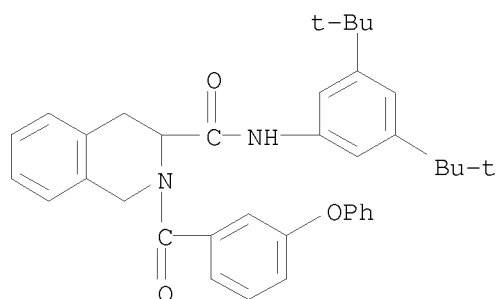
RN 862504-45-8 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(3,4-dimethylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



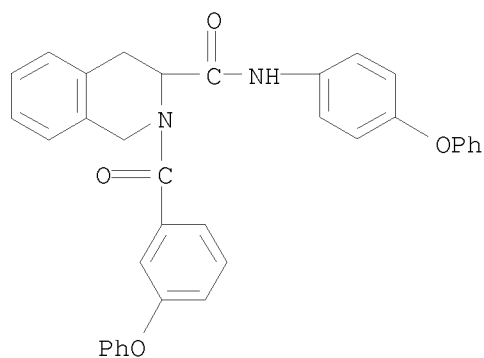
RN 862504-46-9 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[3,5-bis(1,1-dimethylethyl)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



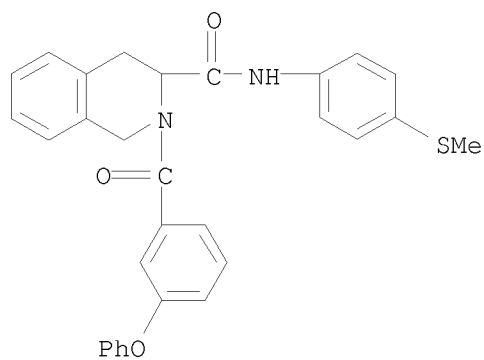
RN 862504-47-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-(4-phenoxyphenyl)- (CA INDEX NAME)



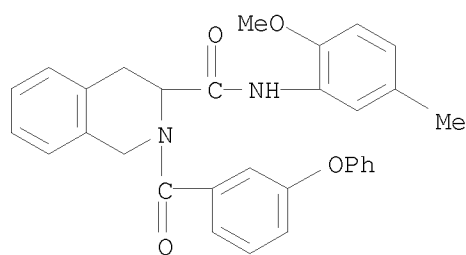
RN 862504-48-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[4-(methylthio)phenyl]-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



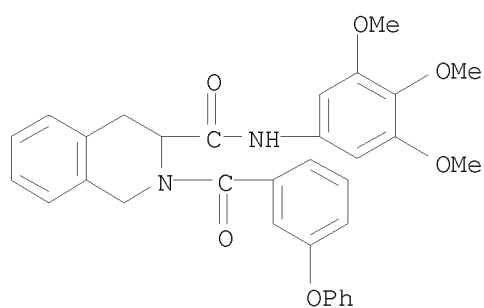
RN 862504-49-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(2-methoxy-5-methylphenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



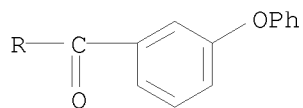
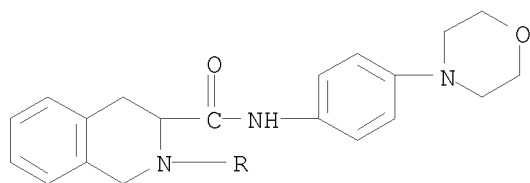
RN 862504-50-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



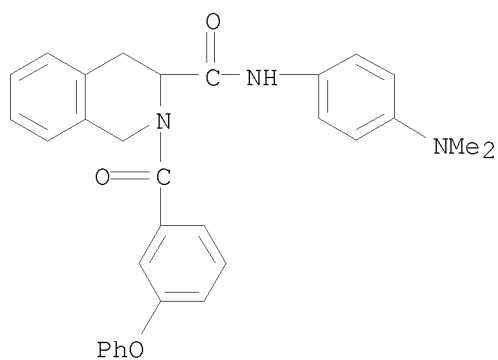
RN 862504-51-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[4-(4-morpholinyl)phenyl]-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



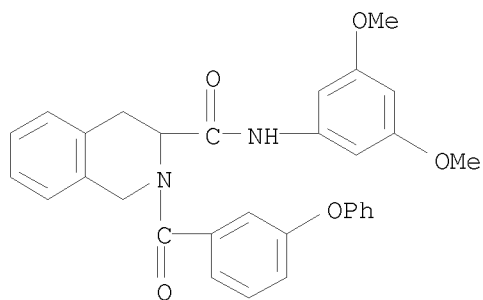
RN 862504-52-7 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-(dimethylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



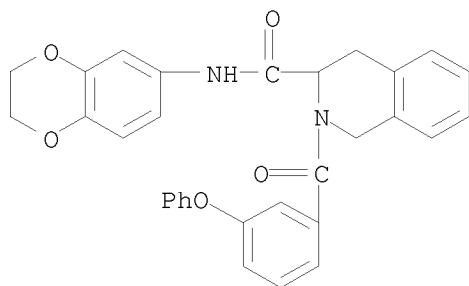
RN 862504-53-8 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(3,5-dimethoxyphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



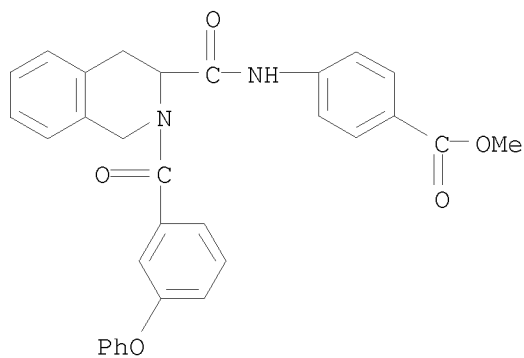
RN 862504-54-9 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



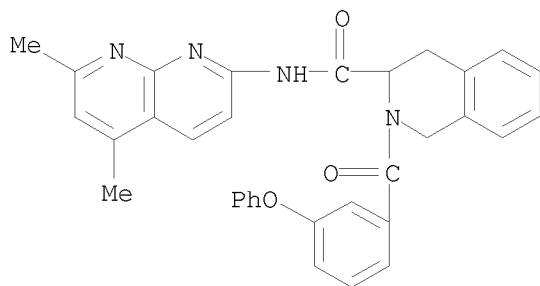
RN 862504-55-0 CAPLUS

CN Benzoic acid, 4-[[[1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-3-isoquinolinyl]carbonyl]amino]-, methyl ester (CA INDEX NAME)



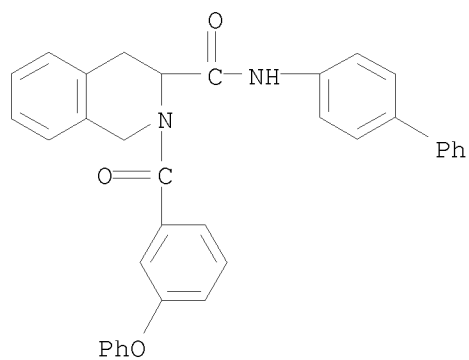
RN 862504-56-1 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(5,7-dimethyl-1,8-naphthyridin-2-yl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



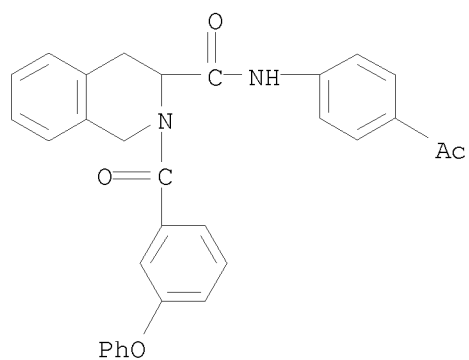
RN 862504-57-2 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[1,1'-biphenyl]-4-yl-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



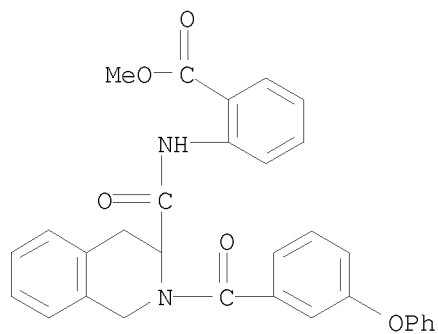
RN 862504-58-3 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-acetylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862504-59-4 CAPLUS

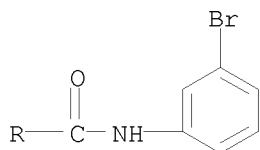
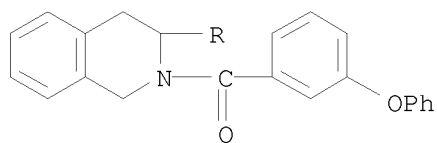
CN Benzoic acid, 2-[[[1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-3-isoquinolinyl]carbonyl]amino]-, methyl ester (CA INDEX NAME)



RN 862504-60-7 CAPLUS

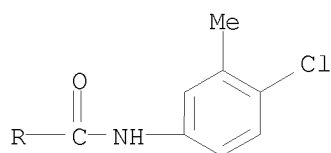
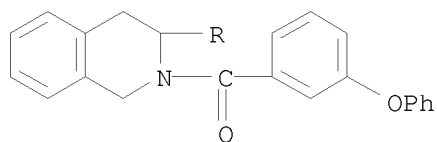
CN 3-Isoquinolinecarboxamide, N-(3-bromophenyl)-1,2,3,4-tetrahydro-2-(3-

phenoxybenzoyl)- (CA INDEX NAME)



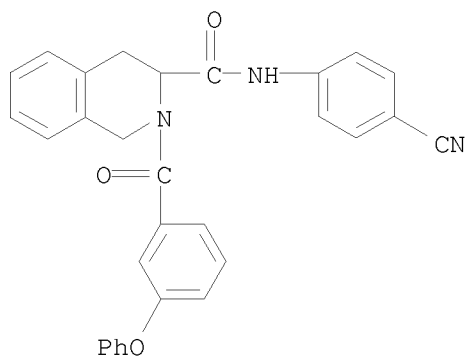
RN 862504-61-8 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chloro-3-methylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



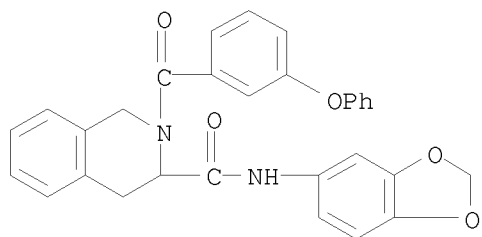
RN 862504-63-0 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-cyanophenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



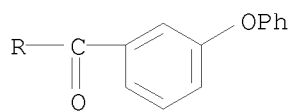
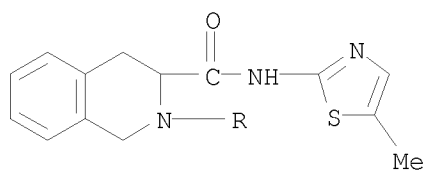
RN 862504-64-1 CAPLUS

CN 3-Isoquinolinecarboxamide, N-1,3-benzodioxol-5-yl-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



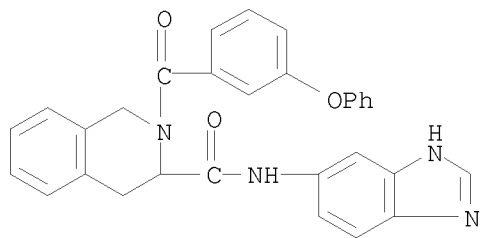
RN 862504-65-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(5-methyl-2-thiazolyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



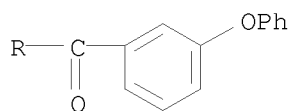
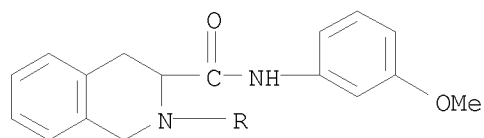
RN 862504-66-3 CAPLUS

CN 3-Isoquinolinecarboxamide, N-1H-benzimidazol-6-yl-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)

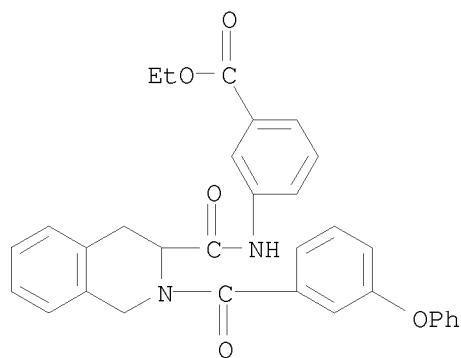


RN 862504-67-4 CAPLUS

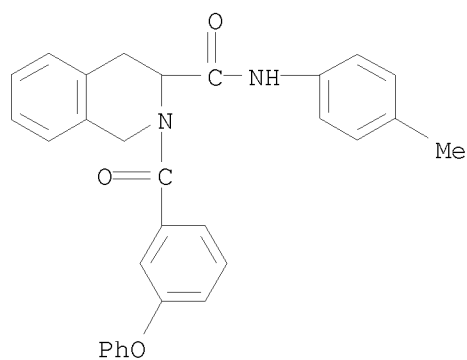
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(3-methoxyphenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862504-68-5 CAPLUS
 CN Benzoic acid, 3-[[[1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-3-isoquinolinyl]carbonyl]amino]-, ethyl ester (CA INDEX NAME)

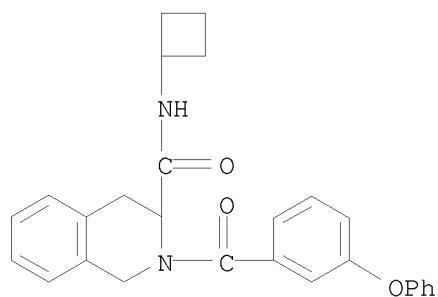


RN 862504-69-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-methylphenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



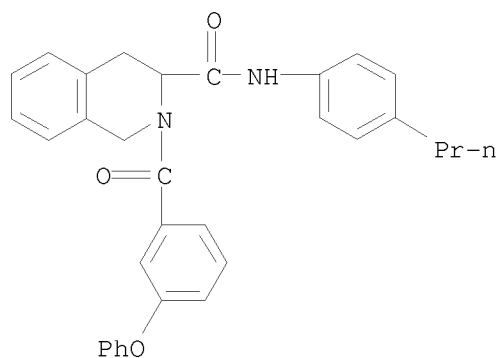
RN 862504-78-7 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-cyclobutyl-1,2,3,4-tetrahydro-2-(3-

phenoxybenzoyl)- (CA INDEX NAME)



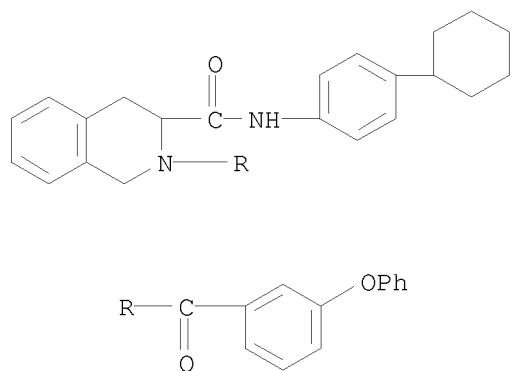
RN 862504-81-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-(4-propylphenyl)- (CA INDEX NAME)



RN 862504-84-5 CAPLUS

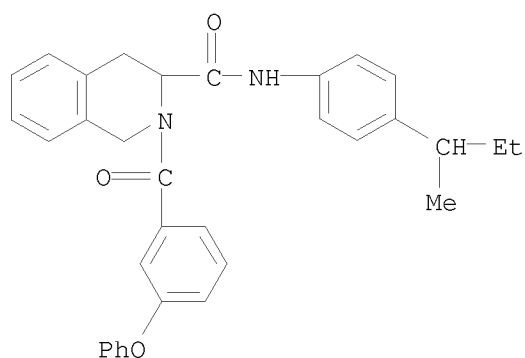
CN 3-Isoquinolinecarboxamide, N-(4-cyclohexylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862504-87-8 CAPLUS

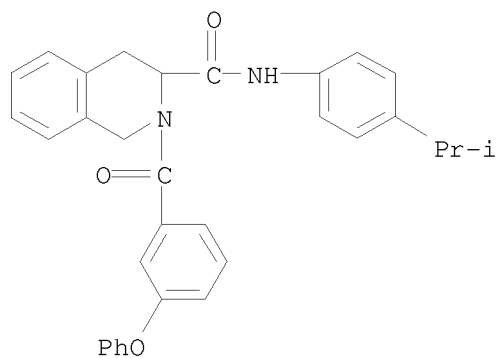
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[4-(1-methylpropyl)phenyl]-

2-(3-phenoxybenzoyl)- (CA INDEX NAME)



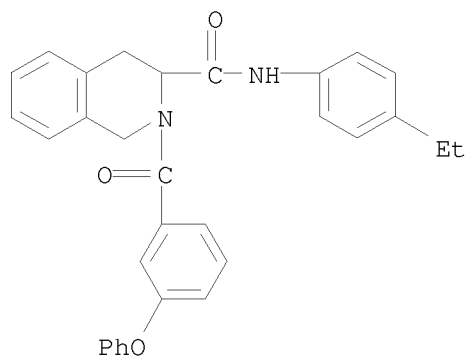
RN 862504-90-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[4-(1-methylethyl)phenyl]-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



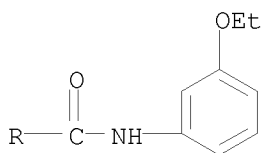
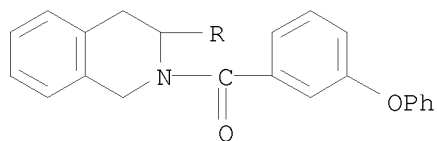
RN 862504-93-6 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-ethylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



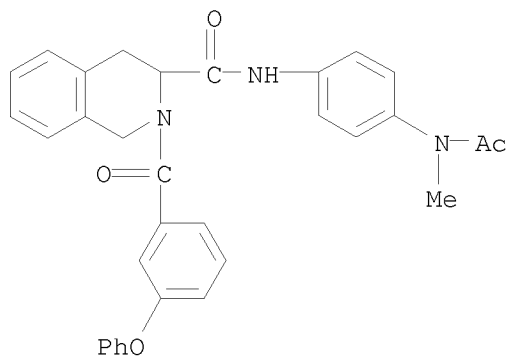
RN 862505-04-2 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(3-ethoxyphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862505-09-7 CAPLUS

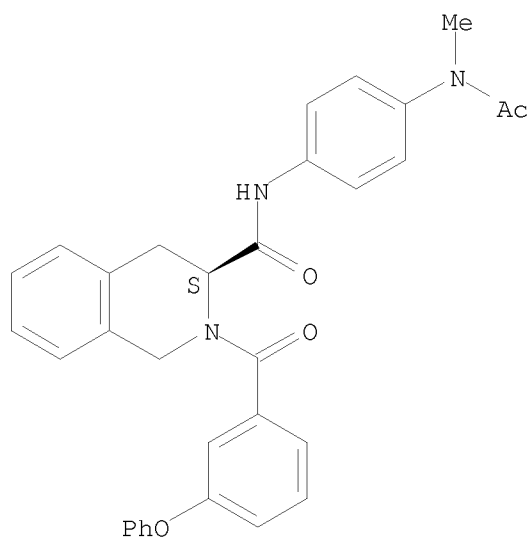
CN 3-Isoquinolinecarboxamide, N-[4-(acetylmethylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862505-12-2 CAPLUS

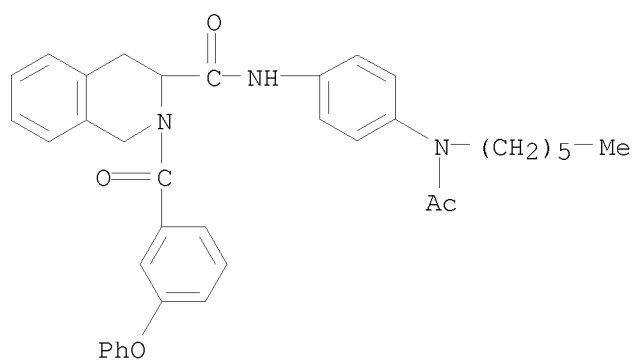
CN 3-Isoquinolinecarboxamide, N-[4-(acetylmethylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 862505-21-3 CAPLUS

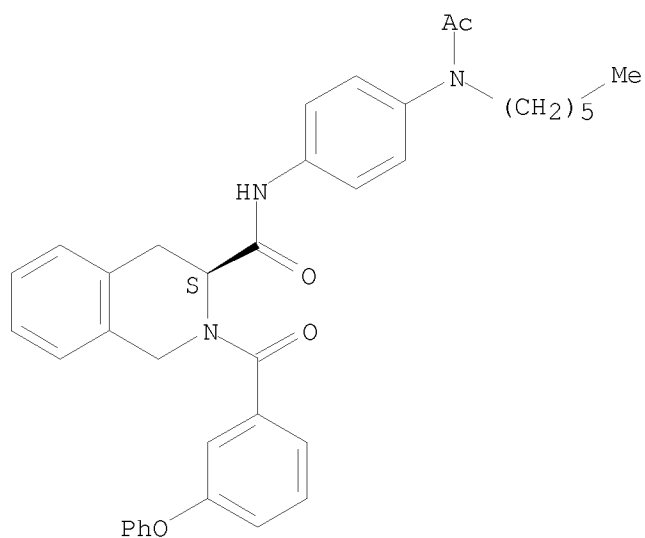
CN 3-Isoquinolinecarboxamide, N-[4-(acetylhexylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862505-24-6 CAPLUS

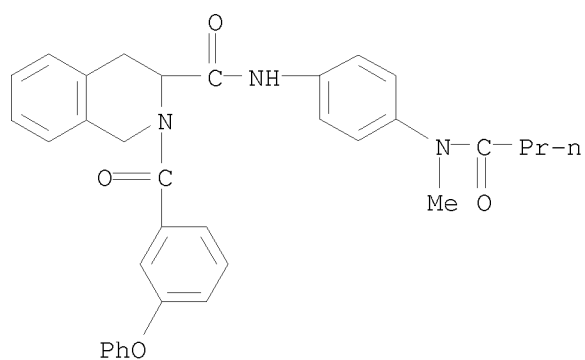
CN 3-Isoquinolinecarboxamide, N-[4-(acetylhexylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



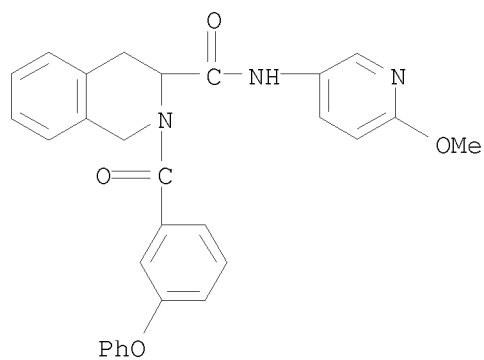
RN 862505-33-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[4-[methyl(1-oxobutyl)amino]phenyl]-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



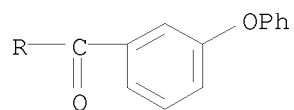
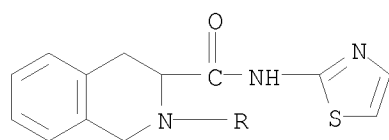
RN 862505-42-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(6-methoxy-3-pyridinyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 862505-45-1 CAPLUS

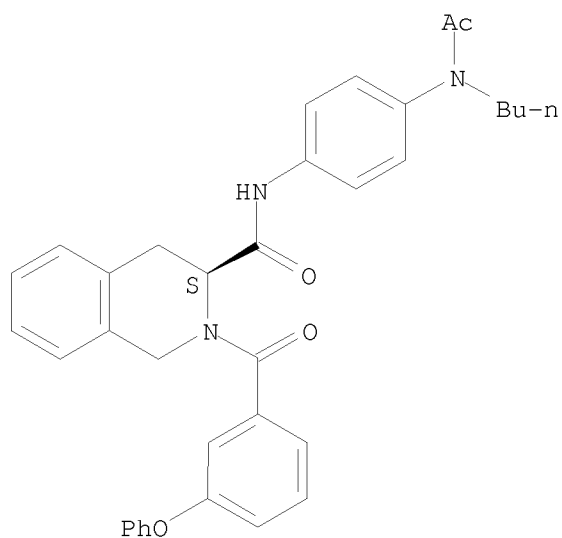
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-2-thiazolyl- (CA INDEX NAME)



RN 862505-52-0 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-(acetylbutylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

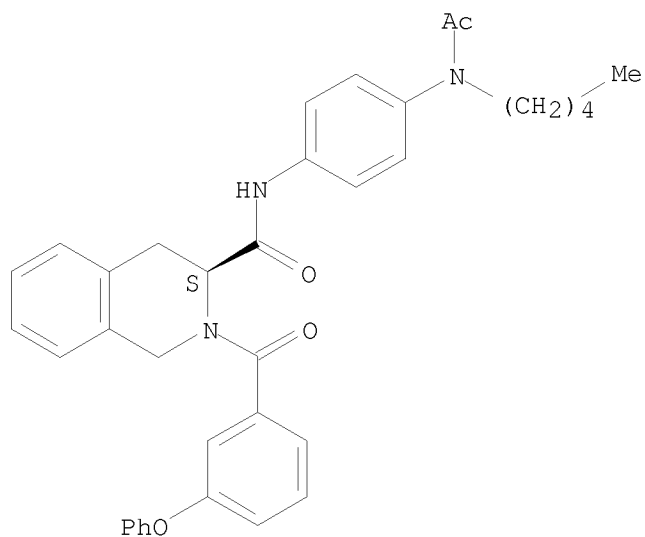
Absolute stereochemistry.



RN 862505-57-5 CAPLUS

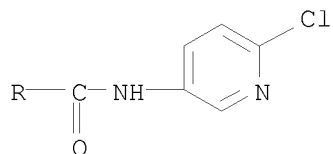
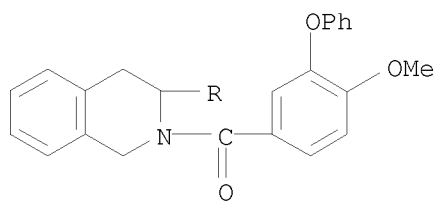
CN 3-Isoquinolinecarboxamide, N-[4-(acetylpentylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



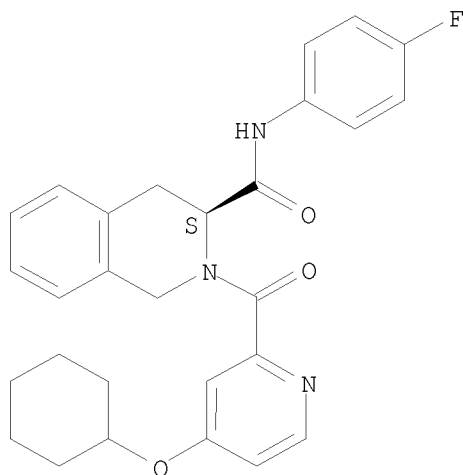
RN 862505-64-4 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(6-chloro-3-pyridinyl)-1,2,3,4-tetrahydro-2-(4-methoxy-3-phenoxybenzoyl)- (CA INDEX NAME)



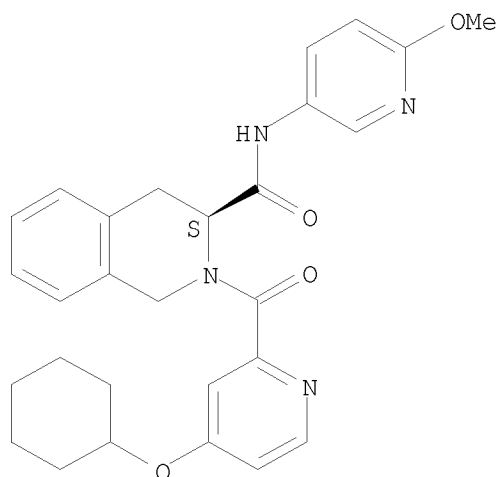
RN 862505-65-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[[4-(cyclohexyloxy)-2-pyridinyl]carbonyl]-N-(4-fluorophenyl)-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 862505-68-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[[4-(cyclohexyloxy)-2-pyridinyl]carbonyl]-1,2,3,4-tetrahydro-N-(6-methoxy-3-pyridinyl)-, (3S)- (CA INDEX NAME)

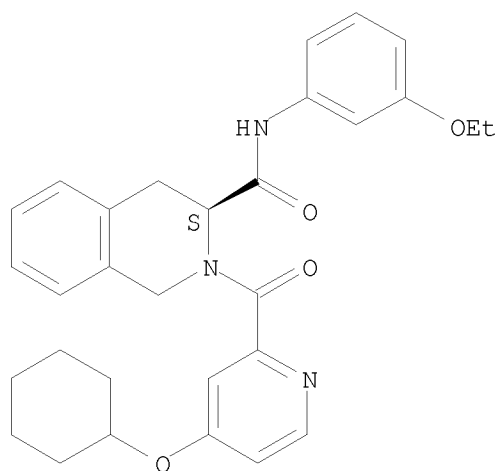
Absolute stereochemistry.



RN 862505-71-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[[4-(cyclohexyloxy)-2-pyridinyl]carbonyl]-N-(3-ethoxyphenyl)-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

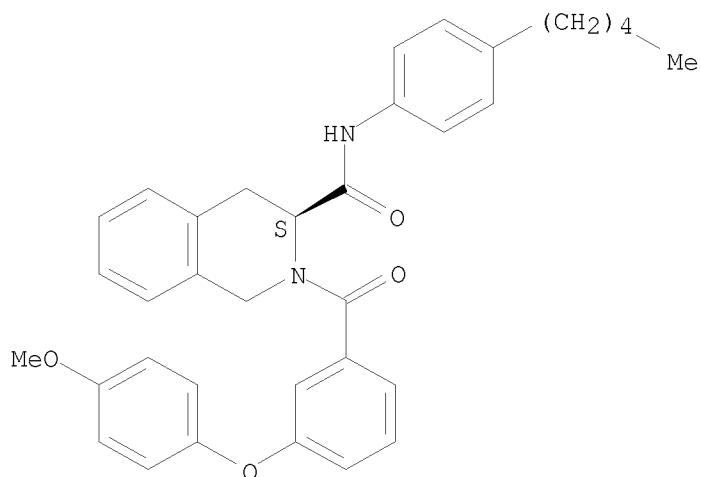
Absolute stereochemistry.



RN 862505-74-6 CAPLUS

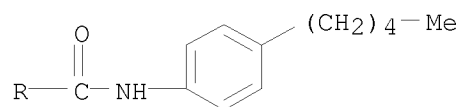
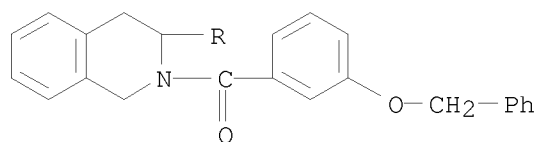
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-methoxyphenoxy)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 862505-77-9 CAPLUS

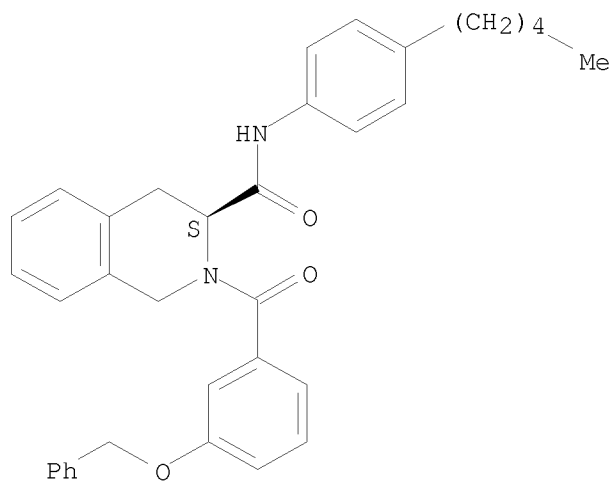
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-[3-(phenylmethoxy)benzoyl]- (CA INDEX NAME)



RN 862505-80-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-[3-(phenylmethoxy)benzoyl]-, (3S)- (CA INDEX NAME)

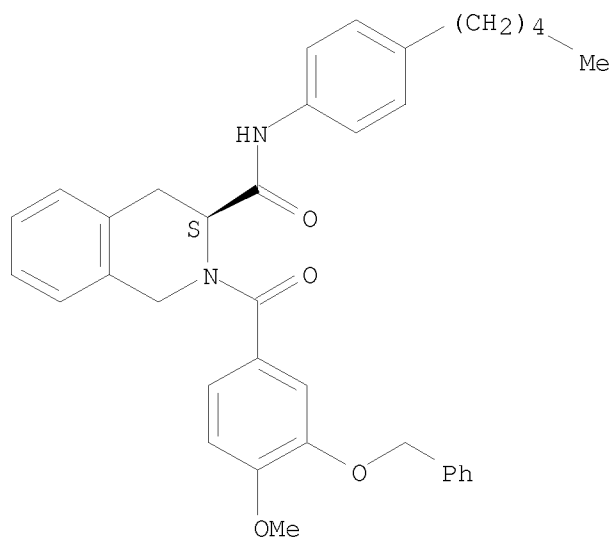
Absolute stereochemistry.



RN 862505-85-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[4-methoxy-3-(phenylmethoxy)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

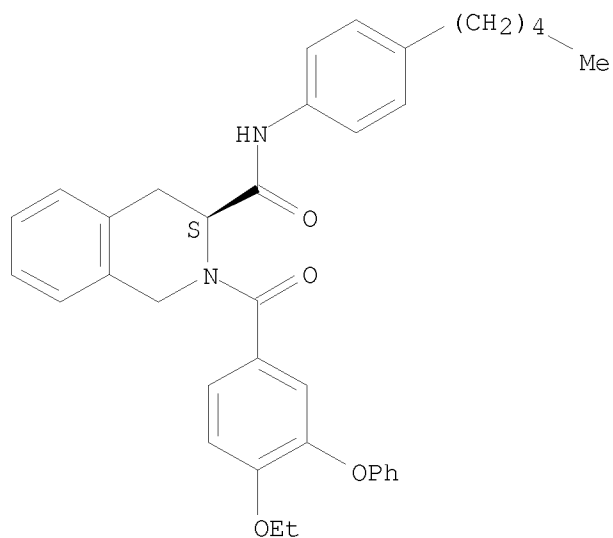
Absolute stereochemistry.



RN 862505-96-2 CAPLUS

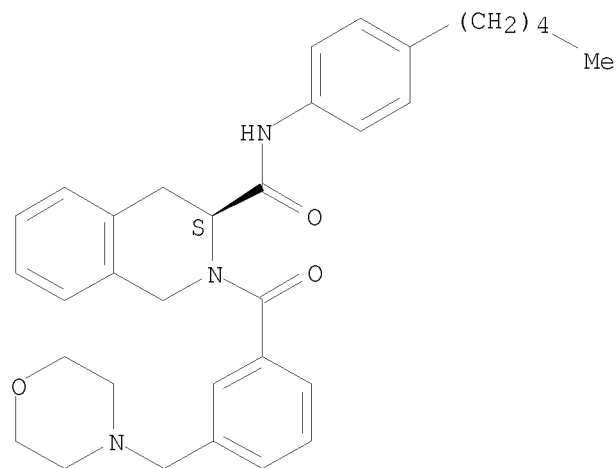
CN 3-Isoquinolinecarboxamide, 2-(4-ethoxy-3-phenoxybenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



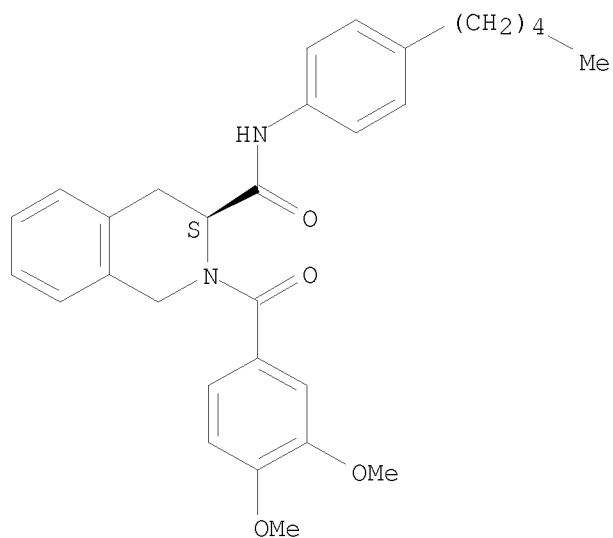
RN 862506-01-2 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinylmethyl)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



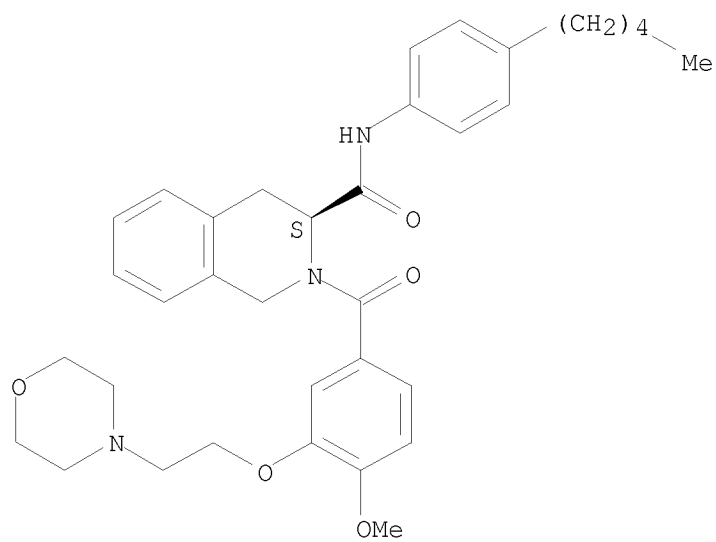
RN 862506-10-3 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-(3,4-dimethoxybenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



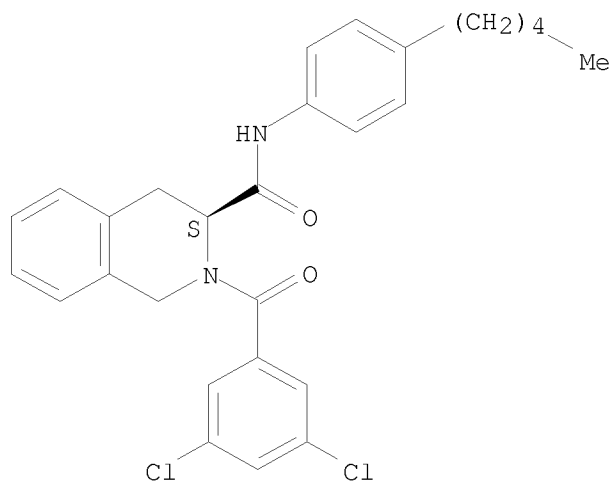
RN 862506-13-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[4-methoxy-3-[2-(4-morpholinyl)ethoxy]benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 862506-24-9 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-(3,5-dichlorobenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

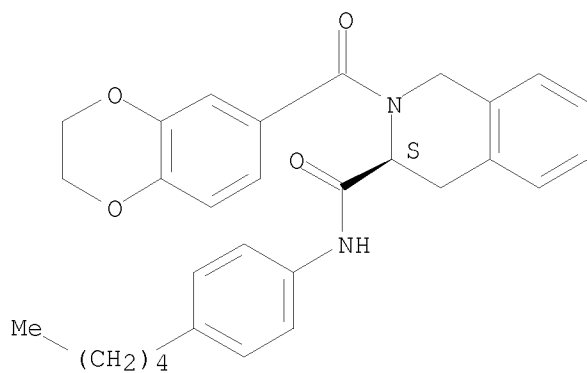
Absolute stereochemistry.



RN 862506-29-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[(2,3-dihydro-1,4-benzodioxin-6-yl)carbonyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

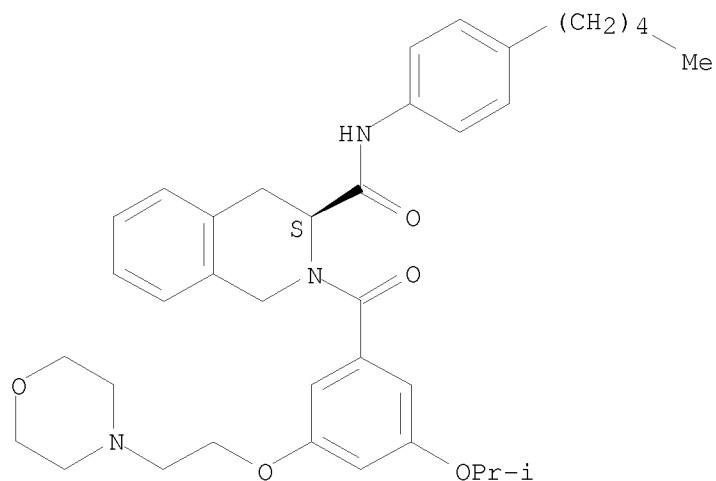
Absolute stereochemistry.



RN 862506-32-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(1-methylethoxy)-5-[2-(4-morpholinyl)ethoxy]benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

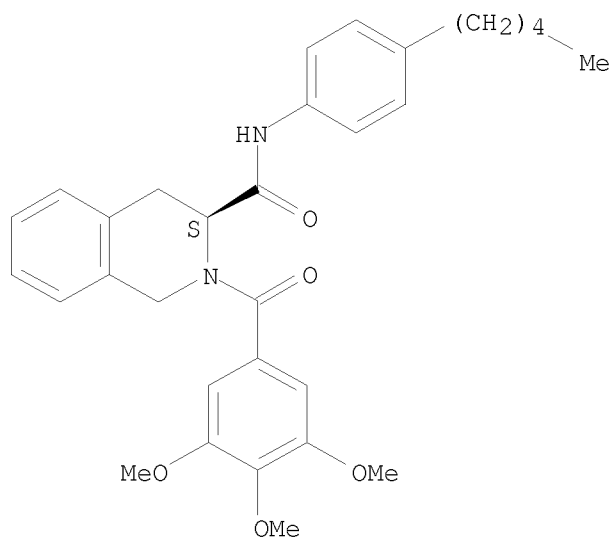
Absolute stereochemistry.



RN 862506-34-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-(3,4,5-trimethoxybenzoyl)-, (3S)- (CA INDEX NAME)

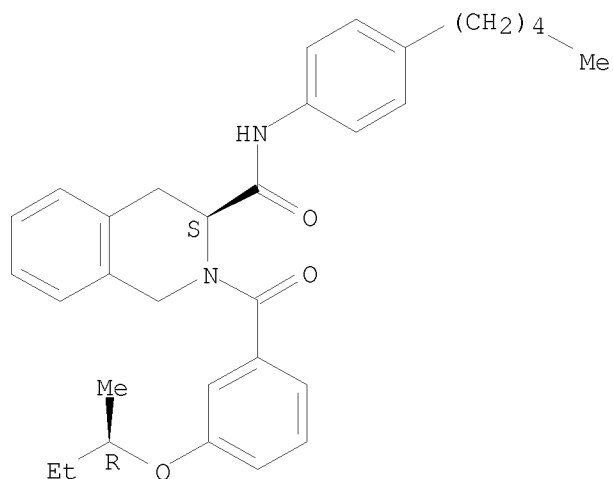
Absolute stereochemistry.



RN 862506-36-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-[(1R)-1-methylpropoxy]benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

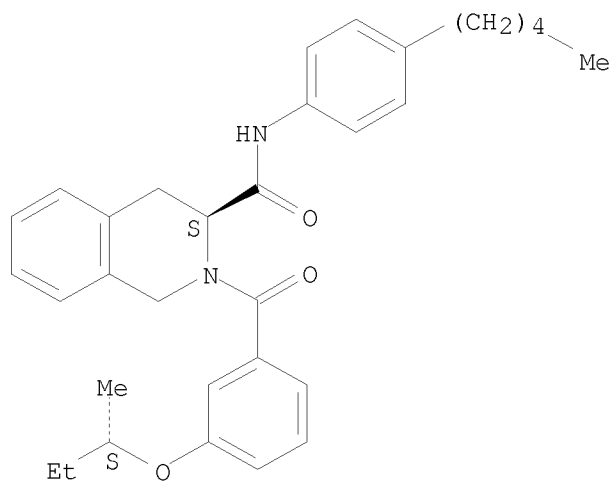
Absolute stereochemistry.



RN 862506-38-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-[(1S)-1-methylpropoxy]benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

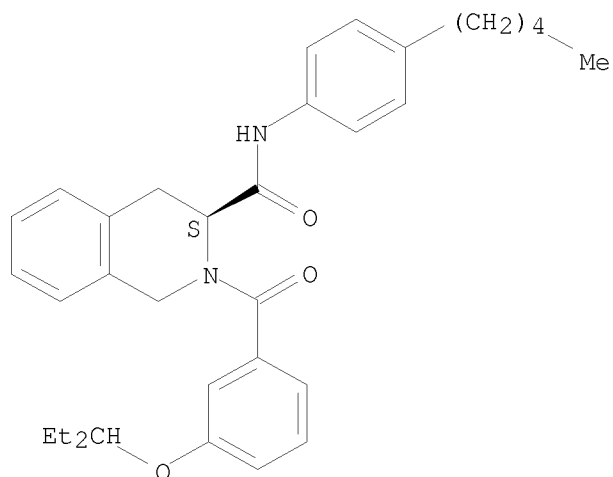
Absolute stereochemistry.



RN 862506-41-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(1-ethylpropoxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

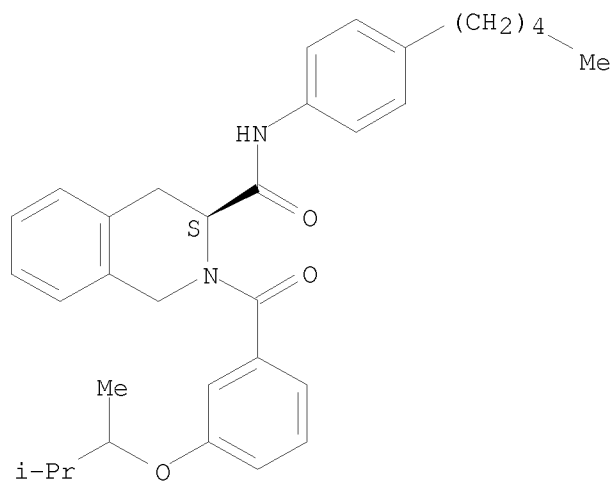
Absolute stereochemistry.



RN 862506-44-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(1,2-dimethylpropoxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

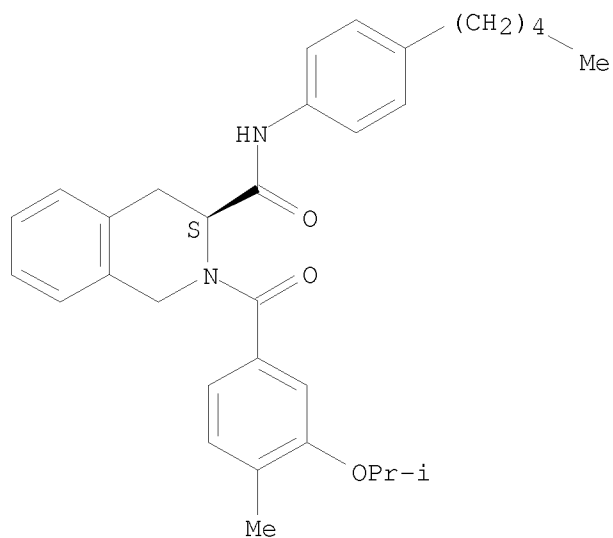
Absolute stereochemistry.



RN 862506-47-6 CAPLUS

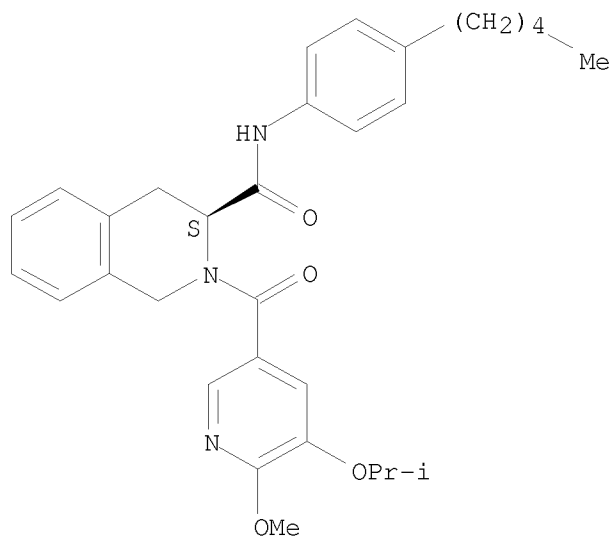
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[4-methyl-3-(1-methylethoxy)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



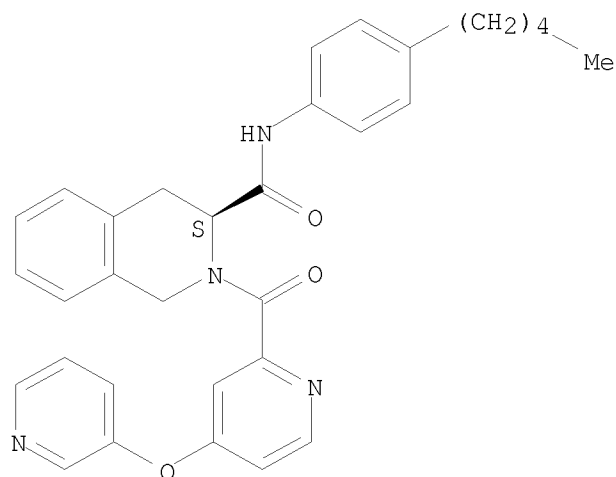
RN 862506-52-3 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[6-methoxy-5-(1-methylethoxy)-3-pyridinyl]carbonyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



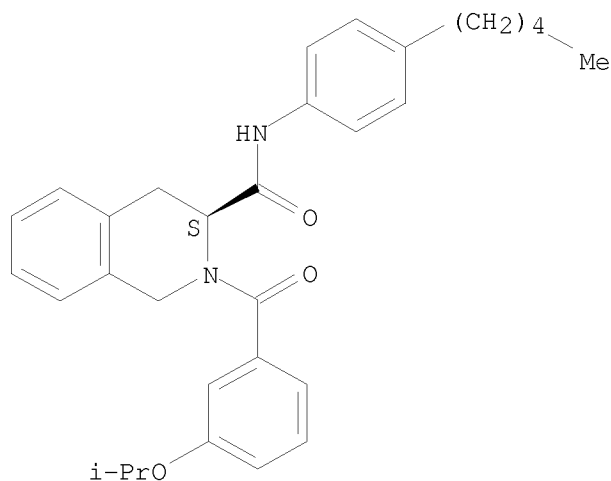
RN 862506-57-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-[[4-(3-pyridinyloxy)-2-pyridinyl]carbonyl]-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 851777-78-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of tetrahydroisoquinoline derivs. for treating diseases
 mediated by protein trafficking or chloride channel activity)
 RN 851777-78-1 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(1-
 methylethoxy)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

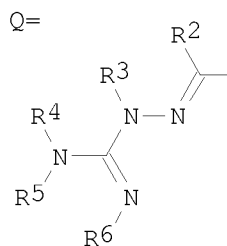
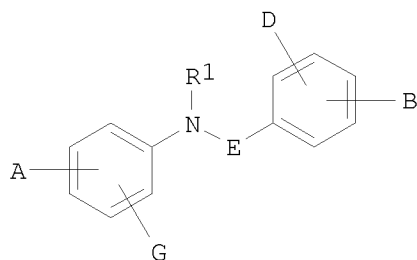
Absolute stereochemistry.



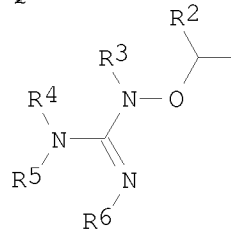
L4 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:395032 CAPLUS
 DOCUMENT NUMBER: 142:447228
 TITLE: Preparation of acetophenone guanylylhydrazone compounds
 as inhibitors of RNase P proteins and antibacterial
 compounds
 INVENTOR(S): Powers, Gordon D.; Sturgess, Michael A.

PATENT ASSIGNEE(S): Message Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 78 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

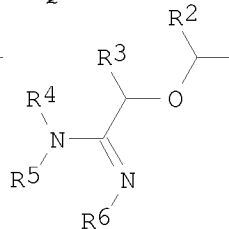
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005039494	A2	20050506	WO 2004-US34839	20041021
WO 2005039494	A3	20050721		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050187409	A1	20050825	US 2004-970190	20041021
PRIORITY APPLN. INFO.:			US 2003-512981P	P 20031021
OTHER SOURCE(S):			CASREACT 142:447228; MARPAT 142:447228	
GI				



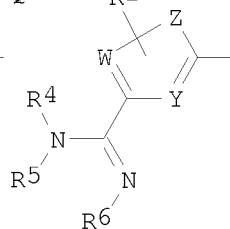
Q1=



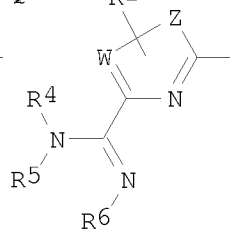
Q2=



Q3=



Q4=



AB Several classes of compds. including mono- and bis-guanylhya zones and benzoic acid compds. (I) [wherein A and B are independently selected from formulas Q-Q4; D and G are independently H, alkyl, aralkyl, heteroalkyl, alkene, heteroalkene, alkyne, heteroalkyne, aryl, heteroaryl, alkoxy,

hydroxy, halogen, amino, nitro, alkylamino, sulfhydryl, or alkylthio; E is C:O, C:S, C:CR8R9, or C:NR7; R1-9 are independently H, alkyl, aryl, or aralkyl; W and Z are independently CH, C-alkyl, or N; and X and Y are independently NH, N-alkyl, O, or S] are prepared. The present invention features compds. useful for inhibiting bacterial RNase P holoenzymes (RNase P activity). These compds. can be used as therapeutics for treating or preventing a variety of bacterial infections. Thus, 4-acetylbenzoic acid was treated with oxalyl chloride in the presence of catalytic amount of DMF in CHCl₃ at room temperature for 2 h and after removing volatiles under vacuum, amidated with 4-aminoacetophenone in the presence of diisopropylethylamine at room temperature overnight to give 4-acetyl-N-(4-acetylphenyl)benzamide which was condensed with aminoguanidine hydrochloride in a mixture of DMSO and ethanolic HCl (a 99:1 mixture of EtOH and concentrated HCl) in a sealed vial at 1105° for 5 days and purified by preparative reverse-phase HPLC using 20,80 MeCN/H₂O (both containing 0.1% CF₃CO₂H) as mobile phase to give bisguanylhyazone of 4-acetyl-N-(4-acetylphenyl)benzamide (II). II showed IC₅₀ of 1 μM against RNase P of bacterium *Neisseria gonorrhoeae*.

IT 851084-06-5P 851084-07-6P 851084-08-7P
851084-09-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acetophenone guanylhyazone compds. as inhibitors of bacterial RNase P holoenzymes and antibacterial compds.)

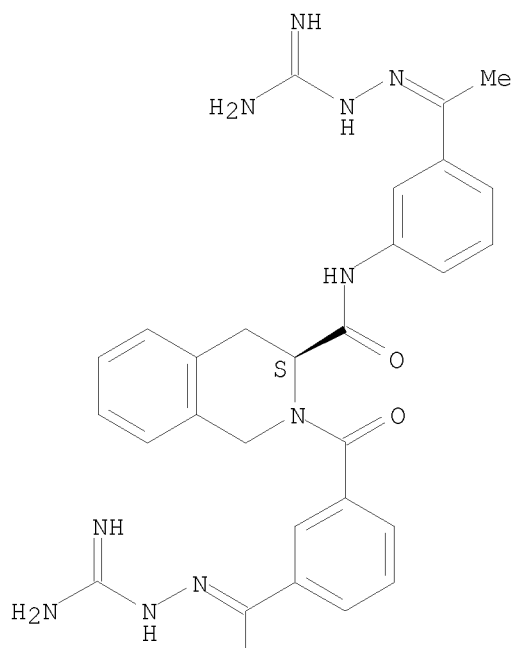
RN 851084-06-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]benzoyl]-N-[3-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]phenyl]-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A



PAGE 2-A



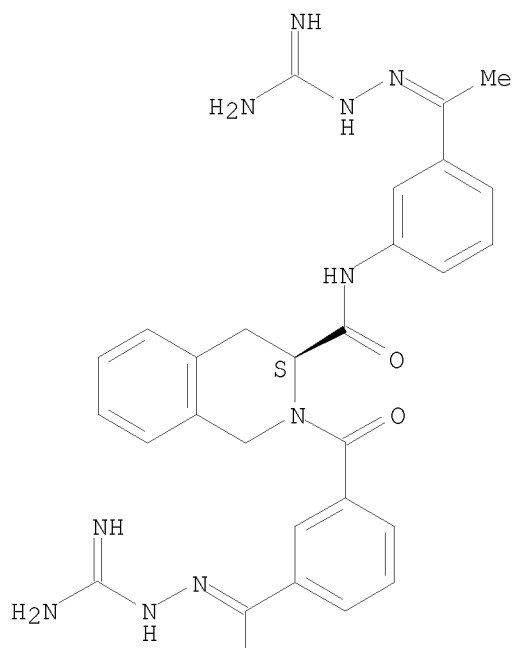
RN 851084-07-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]benzoyl]-N-[3-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]phenyl]-1,2,3,4-tetrahydro-, (3S)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 851084-06-5
 CMF C29 H32 N10 O2

Absolute stereochemistry.
 Double bond geometry unknown.

PAGE 1-A

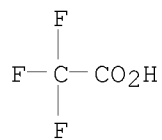


PAGE 2-A



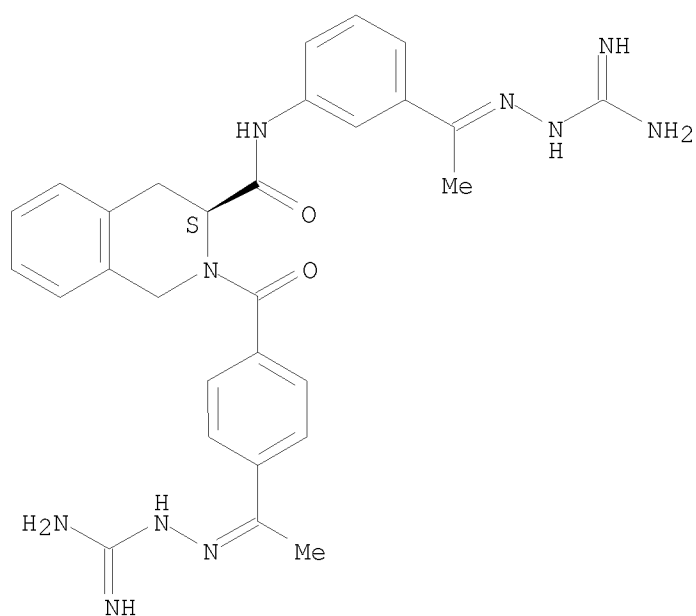
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 851084-08-7 CAPLUS
CN 3-Isoquinolinecarboxamide, 2-[4-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]benzoyl]-N-[3-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]phenyl]-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

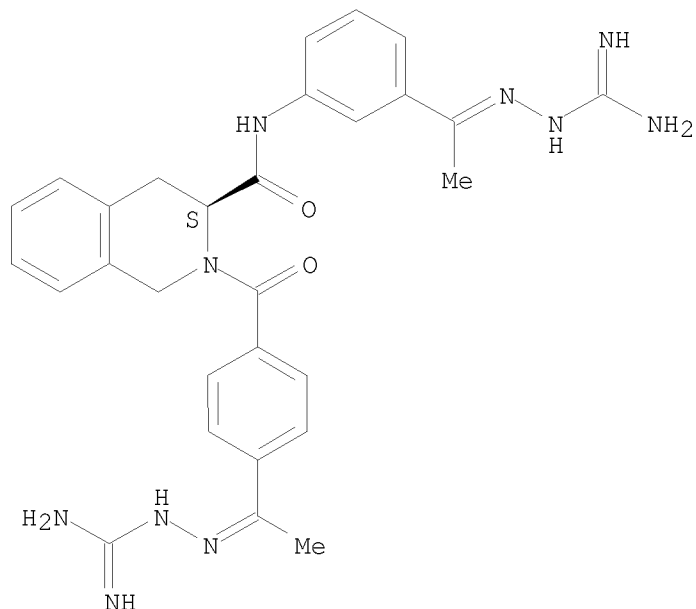


RN 851084-09-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[4-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]benzoyl]-N-[3-[1-[2-(aminoiminomethyl)hydrazinylidene]ethyl]phenyl]-1,2,3,4-tetrahydro-, (3S)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

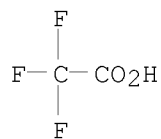
CRN 851084-08-7
 CMF C29 H32 N10 O2

Absolute stereochemistry.
 Double bond geometry unknown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



L4 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:286362 CAPLUS
 DOCUMENT NUMBER: 142:456269
 TITLE: Discovery of 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid diamides that increase CFTR mediated chloride transport
 AUTHOR(S): Hirth, Bradford H.; Qiao, Shuang; Cuff, Lisa M.; Cochran, Brian M.; Pregel, Marko J.; Gregory, Jill S.; Sneddon, Scott F.; Kane, John L.
 CORPORATE SOURCE: Genzyme Corp., Genzyme Drug Discovery and Development, Cambridge, MA, 02139, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(8), 2087-2091
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:456269

AB A series of 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid diamides that increase chloride transport in cells expressing mutant cystic fibrosis transmembrane conductance regulator (CFTR) protein has been identified from our compound library. Analoging efforts and the resulting structure-activity relationships uncovered are detailed. Compound potency was improved over 30-fold from the original lead, yielding several analogs with EC50 values below 10 nM in our cellular chloride transport assay.

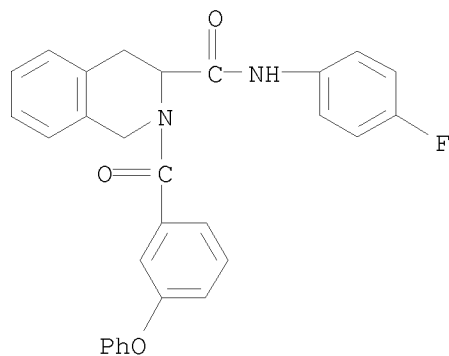
IT 851777-46-3P 851777-47-4P 851777-48-5P
 851777-49-6P 851777-50-9P 851777-51-0P
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 851777-58-7P 851777-59-8P 851777-60-1P
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 851777-94-1P 851777-95-2P

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(discovery of and structure-activity relationship of 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid diamides that increase CFTR mediated chloride transport)

RN 851777-46-3 CAPLUS

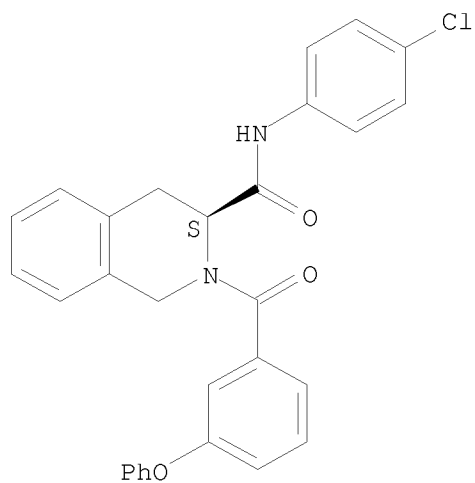
CN 3-Isoquinolinecarboxamide, N-(4-fluorophenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



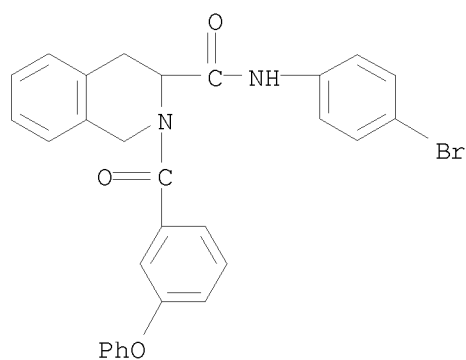
RN 851777-47-4 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

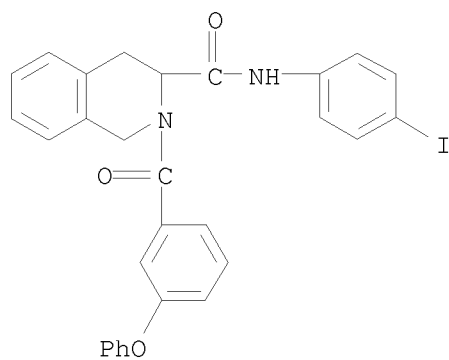
Absolute stereochemistry.



RN 851777-48-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-bromophenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)

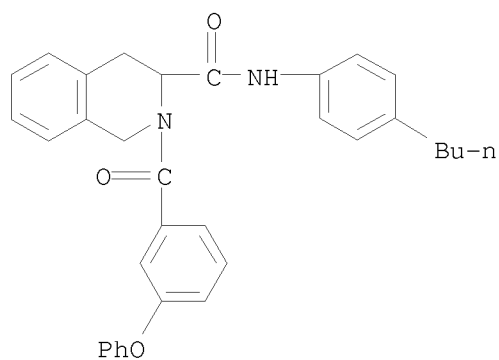


RN 851777-49-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-iodophenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



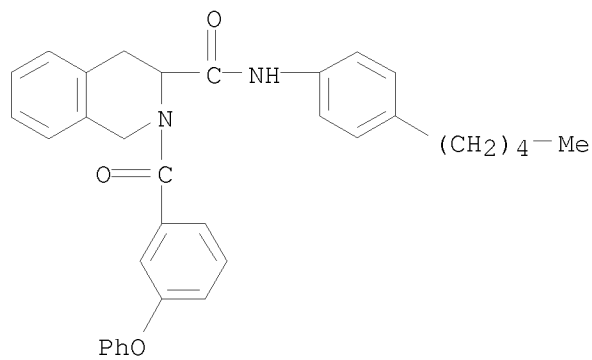
RN 851777-50-9 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-butylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-51-0 CAPLUS

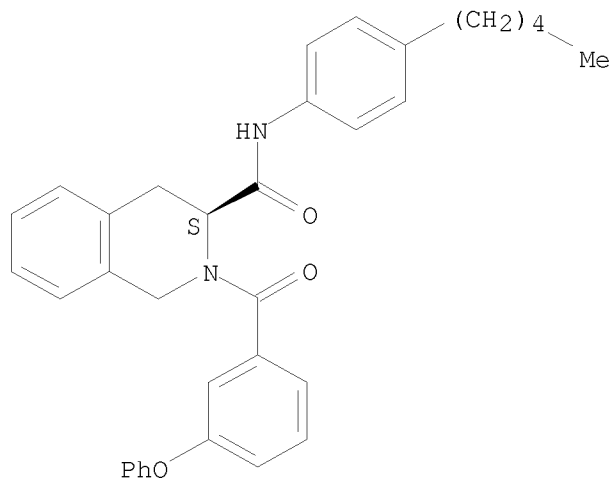
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-52-1 CAPLUS

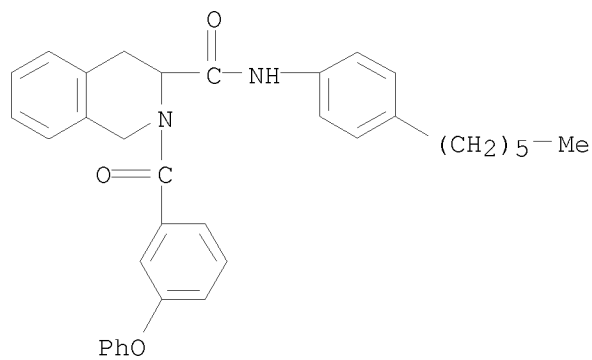
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



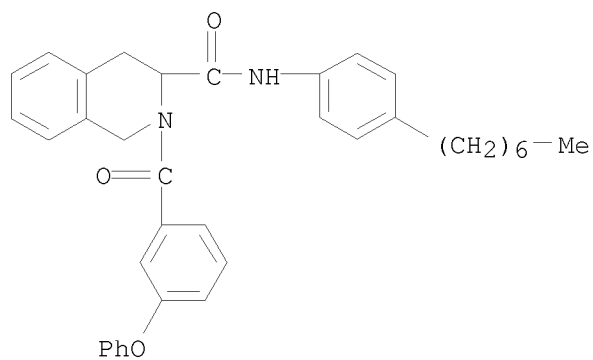
RN 851777-53-2 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-hexylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



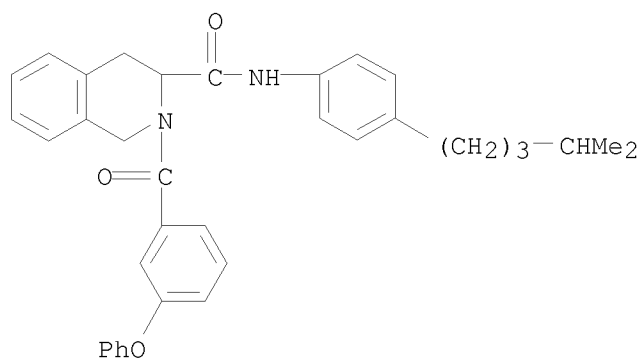
RN 851777-54-3 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-heptylphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



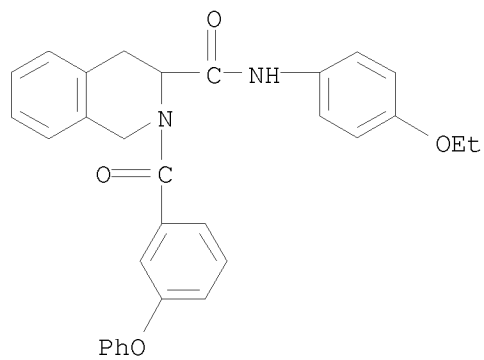
RN 851777-55-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-[4-(4-methylpentyl)phenyl]-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



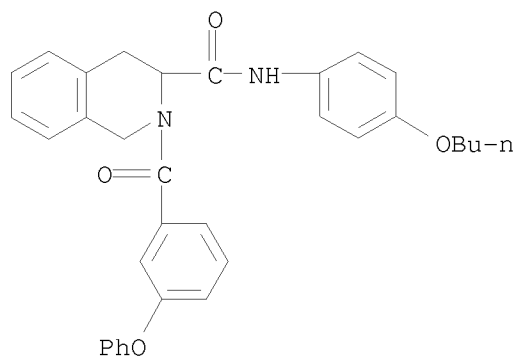
RN 851777-56-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-ethoxyphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



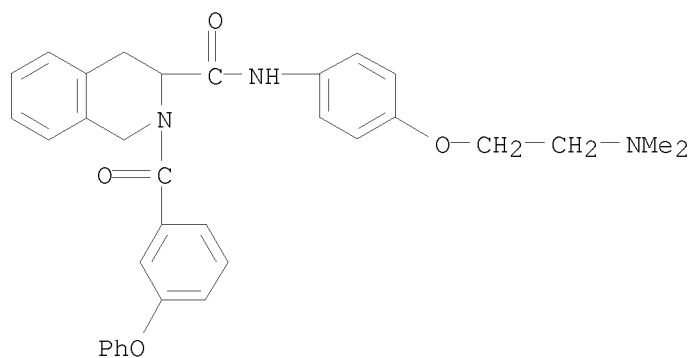
RN 851777-57-6 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-butoxyphenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



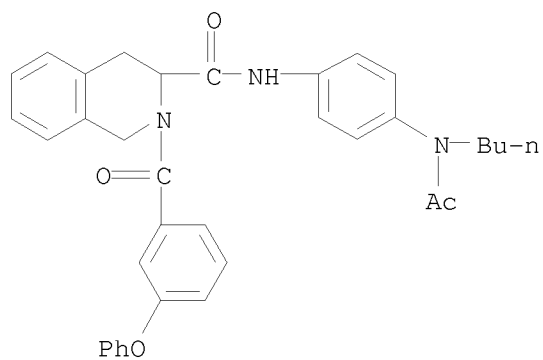
RN 851777-58-7 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-[2-(dimethylamino)ethoxy]phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



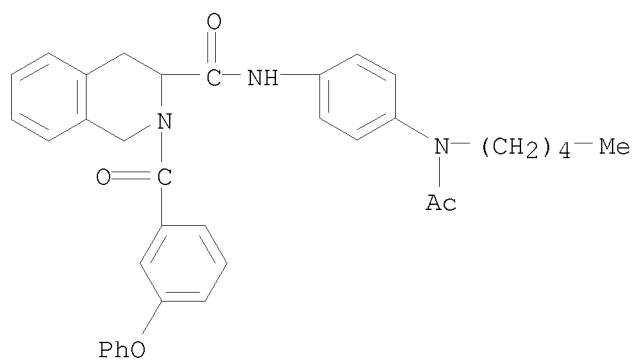
RN 851777-59-8 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-(acetylbutylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



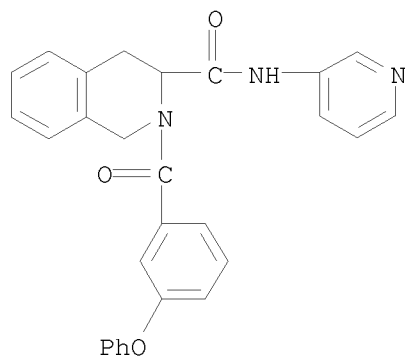
RN 851777-60-1 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[4-(acetylpentylamino)phenyl]-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



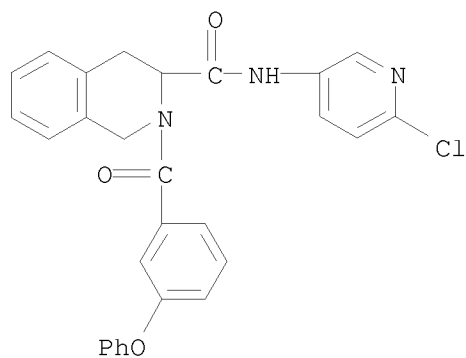
RN 851777-61-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)-N-3-pyridinyl- (CA INDEX NAME)



RN 851777-62-3 CAPLUS

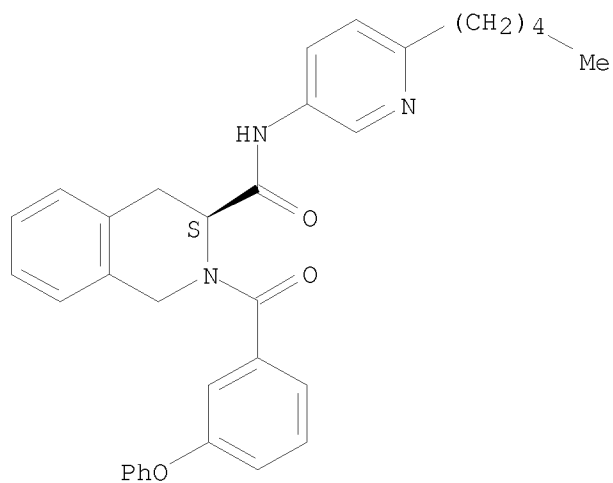
CN 3-Isoquinolinecarboxamide, N-(6-chloro-3-pyridinyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)



RN 851777-63-4 CAPLUS

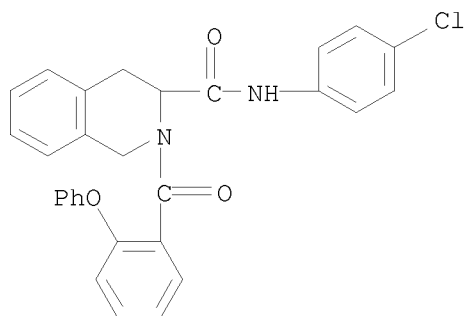
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(6-pentyl-3-pyridinyl)-2-(3-phenoxybenzoyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



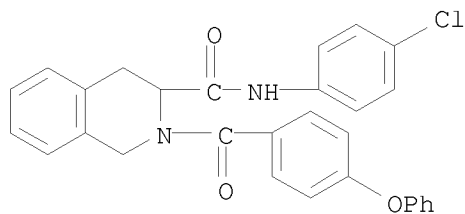
RN 851777-64-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(2-phenoxybenzoyl)- (CA INDEX NAME)



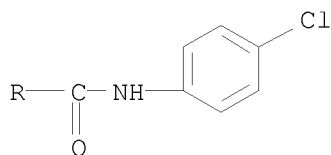
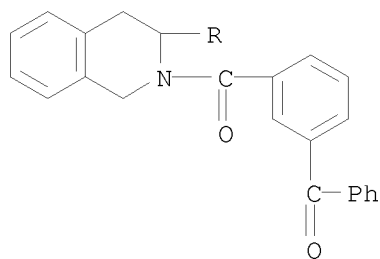
RN 851777-65-6 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(4-phenoxybenzoyl)- (CA INDEX NAME)



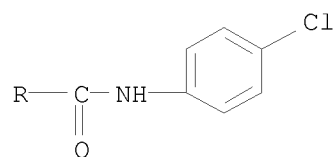
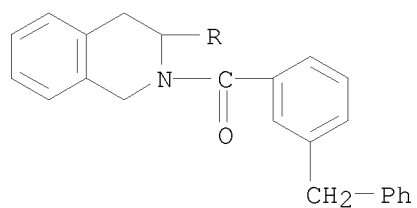
RN 851777-66-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-benzoylbenzoyl)-N-(4-chlorophenyl)-1,2,3,4-tetrahydro- (CA INDEX NAME)



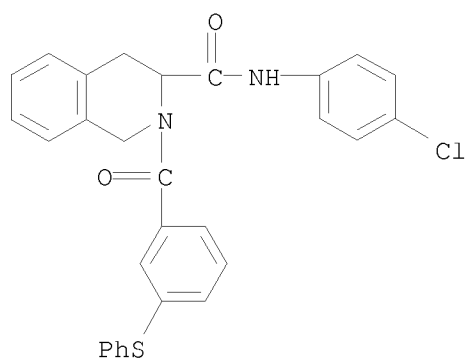
RN 851777-67-8 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(phenylmethyl)benzoyl]- (CA INDEX NAME)



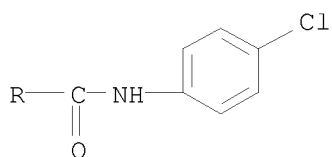
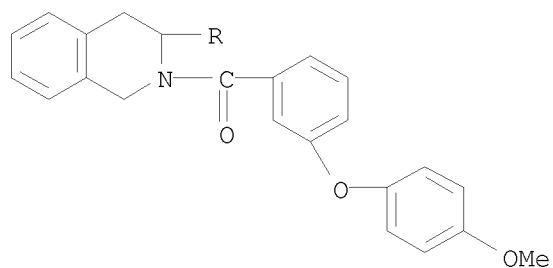
RN 851777-68-9 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(phenylthio)benzoyl]- (CA INDEX NAME)

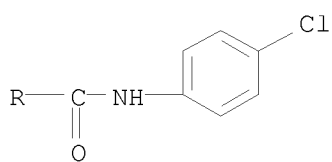
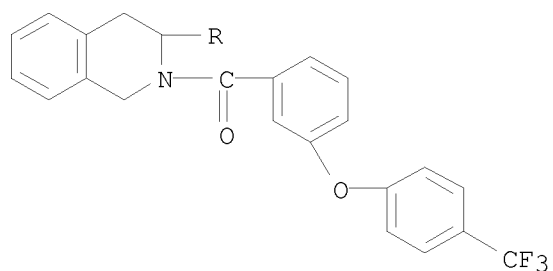


RN 851777-69-0 CAPLUS

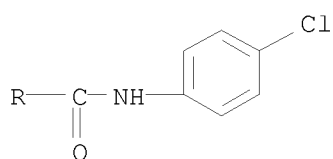
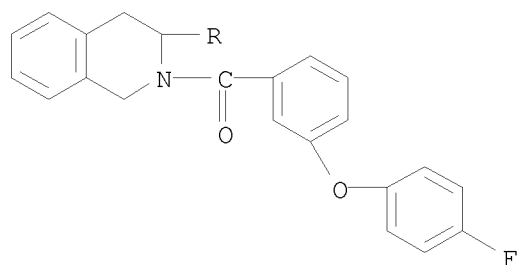
CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(4-methoxyphenoxy)benzoyl]- (CA INDEX NAME)



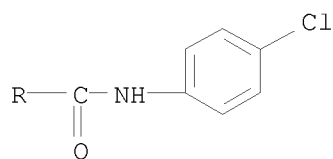
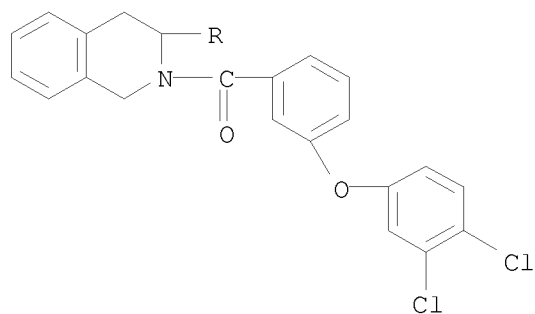
RN 851777-70-3 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-[4-(trifluoromethyl)phenoxy]benzoyl]- (CA INDEX NAME)



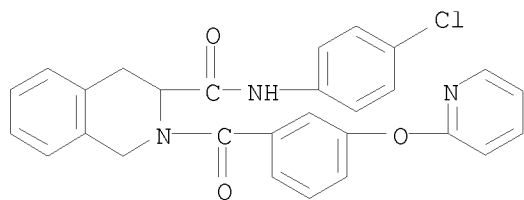
RN 851777-71-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-2-[3-(4-fluorophenoxy)benzoyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



RN 851777-72-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-2-[3-(3,4-dichlorophenoxy)benzoyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



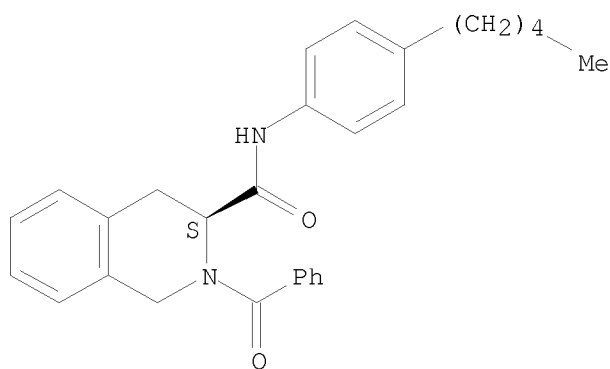
RN 851777-73-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-[3-(2-pyridinyloxy)benzoyl]- (CA INDEX NAME)



RN 851777-74-7 CAPLUS

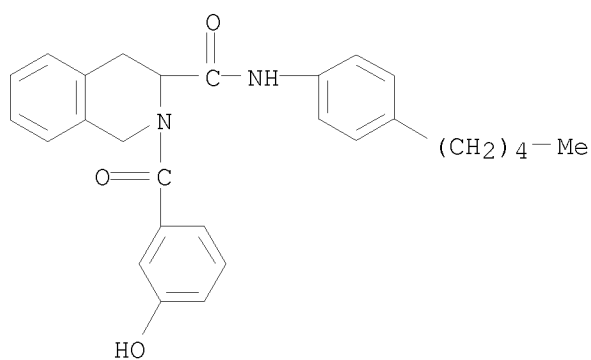
CN 3-Isoquinolinecarboxamide, 2-benzoyl-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 851777-75-8 CAPLUS

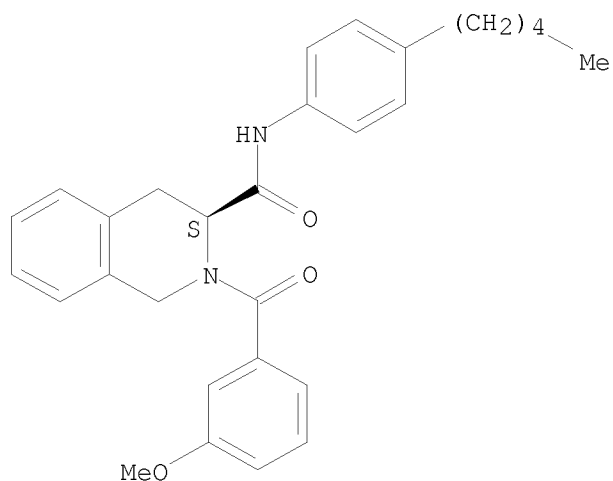
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-hydroxybenzoyl)-N-(4-pentylphenyl)- (CA INDEX NAME)



RN 851777-76-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-methoxybenzoyl)-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

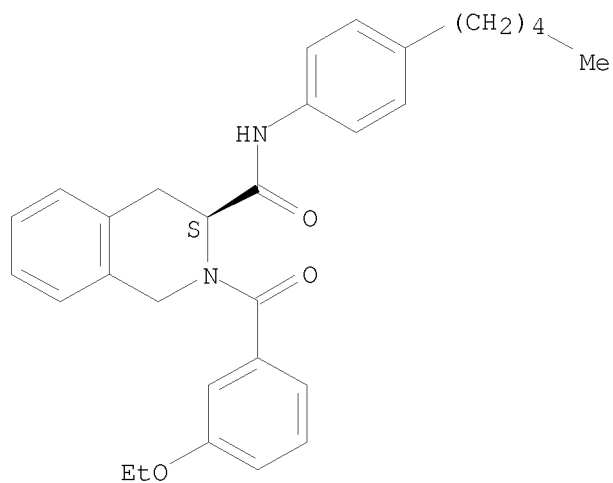
Absolute stereochemistry.



RN 851777-77-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-ethoxybenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

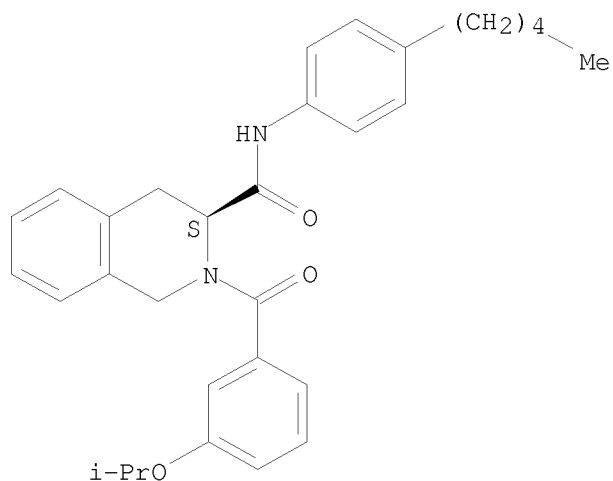
Absolute stereochemistry.



RN 851777-78-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(1-methylethoxy)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

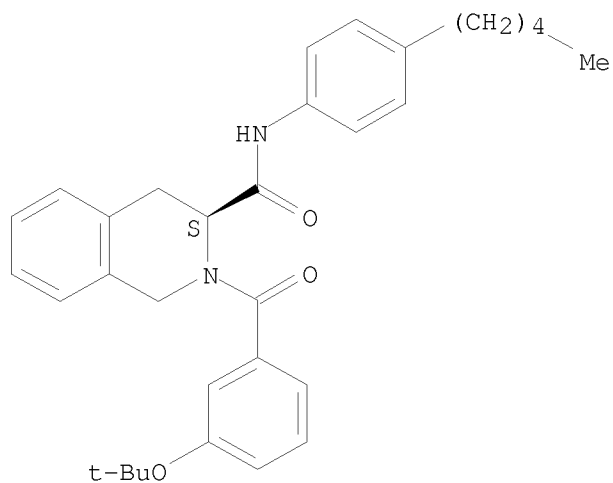
Absolute stereochemistry.



RN 851777-79-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(1,1-dimethylethoxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

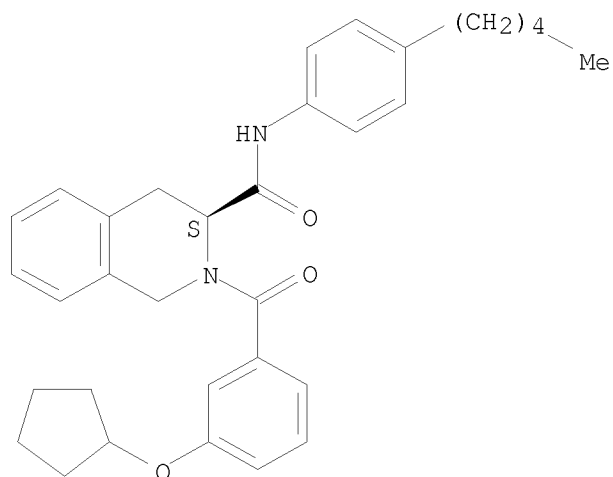
Absolute stereochemistry.



RN 851777-80-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(cyclopentyloxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

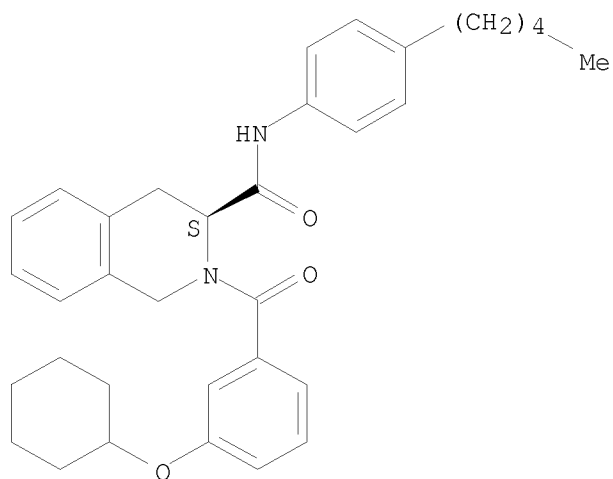
Absolute stereochemistry.



RN 851777-81-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(cyclohexyloxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

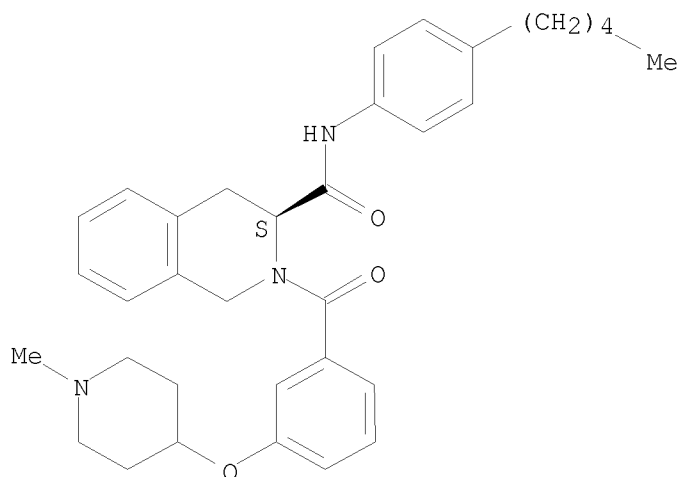
Absolute stereochemistry.



RN 851777-82-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-[(1-methyl-4-piperidinyl)oxy]benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

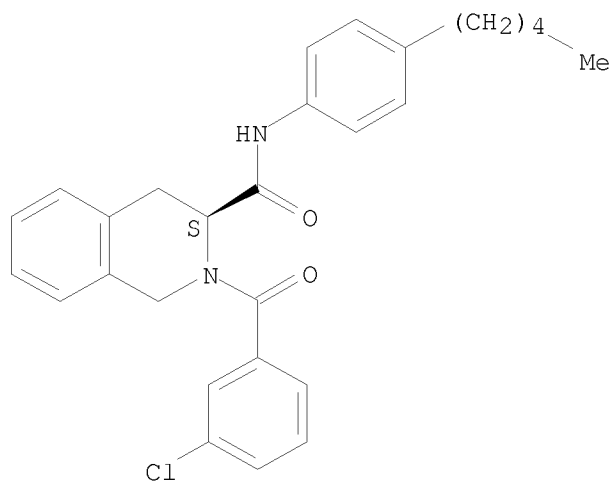
Absolute stereochemistry.



RN 851777-83-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-chlorobenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

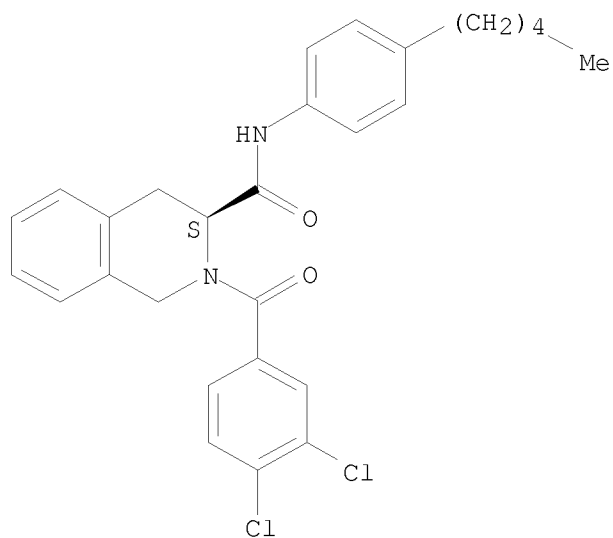
Absolute stereochemistry.



RN 851777-84-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3,4-dichlorobenzoyl)-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

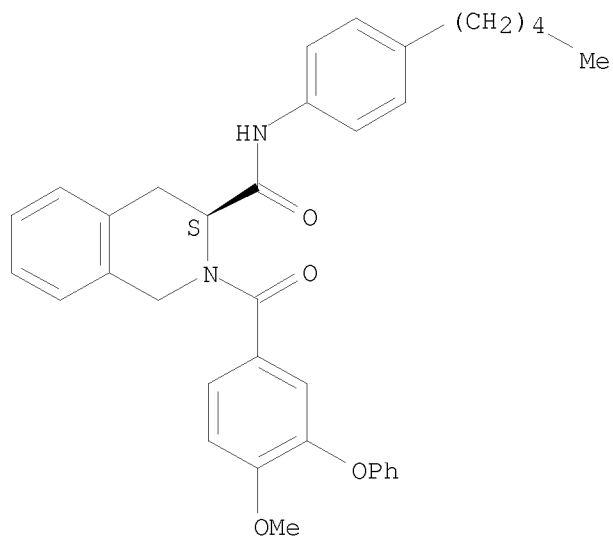
Absolute stereochemistry.



RN 851777-85-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methoxy-3-phenoxycarbonyl)-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

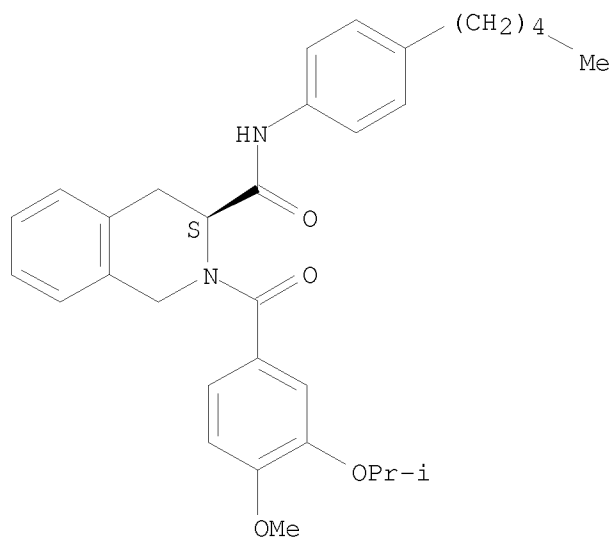
Absolute stereochemistry.



RN 851777-86-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[4-methoxy-3-(1-methylethoxy)benzoyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

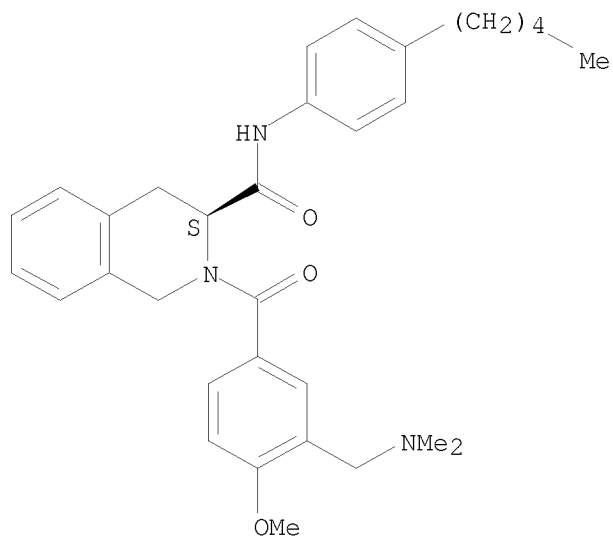
Absolute stereochemistry.



RN 851777-87-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[(dimethylamino)methyl]-4-methoxybenzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

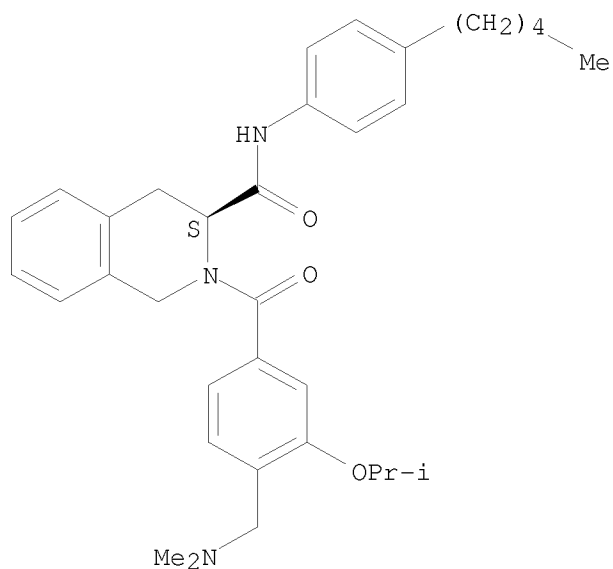
Absolute stereochemistry.



RN 851777-88-3 CAPLUS

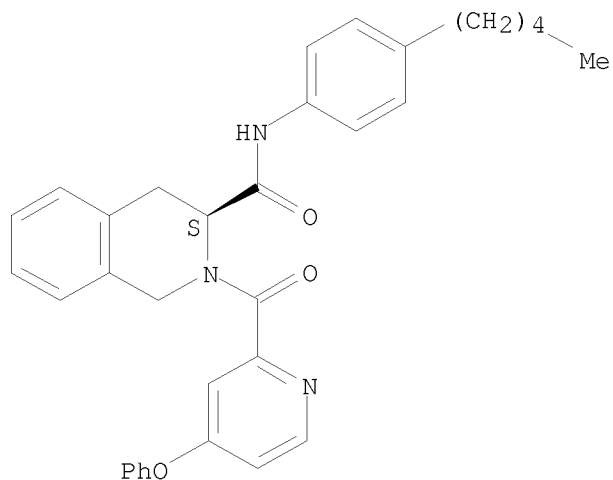
CN 3-Isoquinolinecarboxamide, 2-[4-[(dimethylamino)methyl]-3-(1-methylethoxy)benzoyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



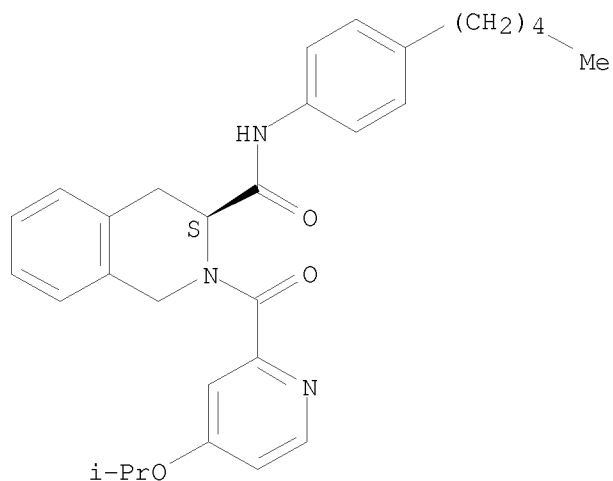
RN 851777-89-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-N-(4-pentylphenyl)-2-[(4-phenoxy-2-pyridinyl)carbonyl]-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 851777-90-7 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[4-(1-methylethoxy)-2-pyridinyl]carbonyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

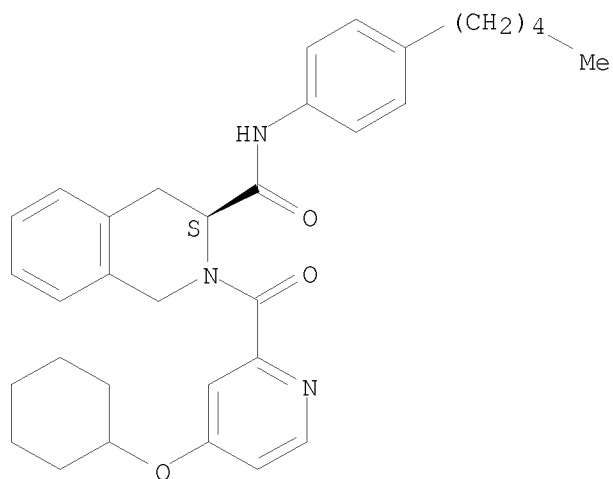
Absolute stereochemistry.



RN 851777-91-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[[4-(cyclohexyloxy)-2-pyridinyl]carbonyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

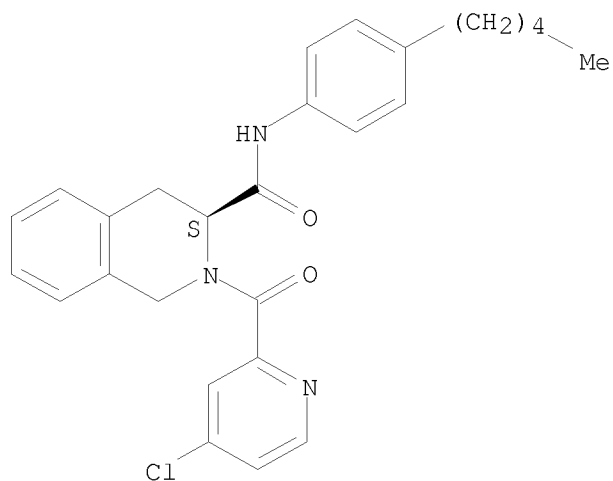
Absolute stereochemistry.



RN 851777-92-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[(4-chloro-2-pyridinyl)carbonyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

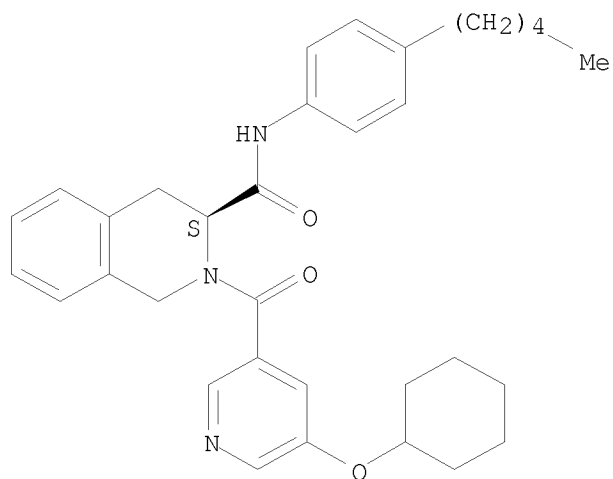
Absolute stereochemistry.



RN 851777-93-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[[5-(cyclohexyloxy)-3-pyridinyl]carbonyl]-1,2,3,4-tetrahydro-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

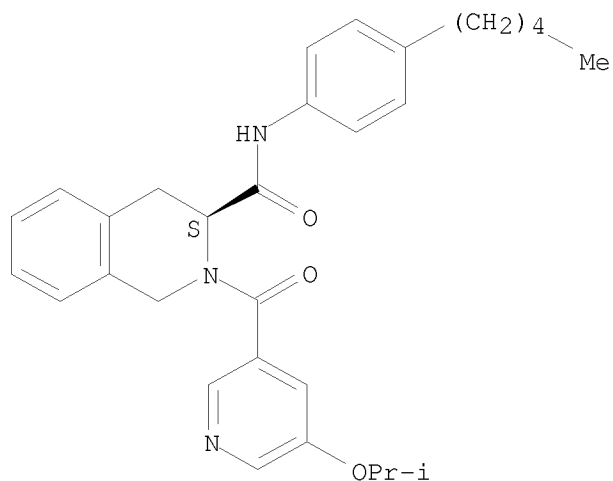
Absolute stereochemistry.



RN 851777-94-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[5-(1-methylethoxy)-3-pyridinyl]carbonyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

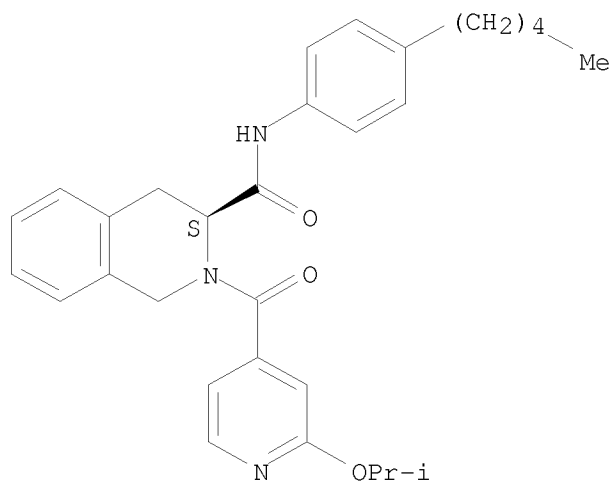
Absolute stereochemistry.



RN 851777-95-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[2-(1-methylethoxy)-4-pyridinyl]carbonyl]-N-(4-pentylphenyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



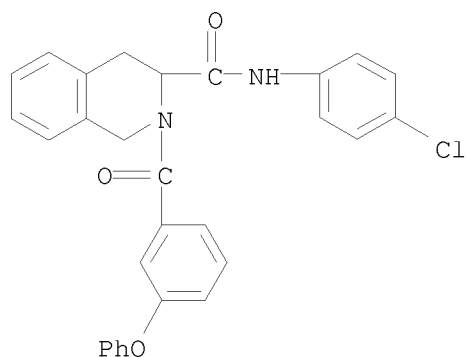
IT 851777-43-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(discovery of and structure-activity relationship of 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid diamides that increase CFTR mediated chloride transport)

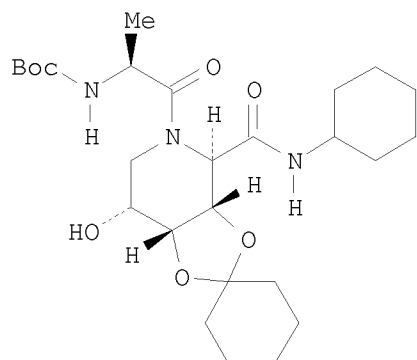
RN 851777-43-0 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(4-chlorophenyl)-1,2,3,4-tetrahydro-2-(3-phenoxybenzoyl)- (CA INDEX NAME)

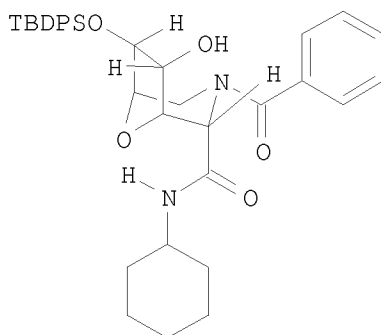


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:74626 CAPLUS
 DOCUMENT NUMBER: 142:298057
 TITLE: Synthesis of functionalized heterocycles via a tandem Staudinger/aza-Wittig/Ugi multicomponent reaction
 AUTHOR(S): Timmer, Mattie S. M.; Risseuw, Martijn D. P.; Verdoes, Martijn; Filippov, Dmitri V.; Plaisier, Jasper R.; Van der Marel, Gijsbert A.; Overkleeft, Herman S.; Van Boom, Jacques H.
 CORPORATE SOURCE: Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden University, Leiden, 2300 RA, Neth.
 SOURCE: Tetrahedron: Asymmetry (2005), 16(1), 177-185
 CODEN: TASYE3; ISSN: 0957-4166
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:298057
 GI



I



II

AB By combining a Staudinger/aza-Wittig and an Ugi three-component reaction in a one-pot process, an efficient multicomponent reaction was developed.

The application of this reaction on readily available azido-aldehydes gave easy access to highly functionalized, enantiomerically pure pipecolic acid amides, e.g., I, and bridged morpholine amide derivs., e.g., II. The versatility of this methodol. was demonstrated by the construction of a mol. library.

IT 847740-12-9P

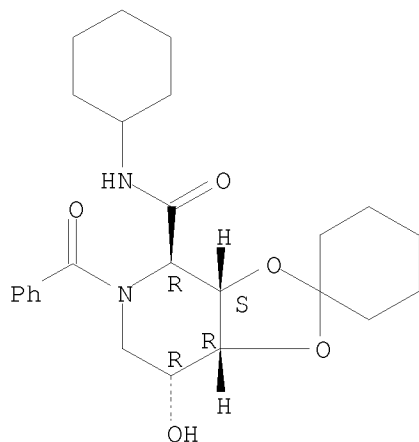
RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective preparation of functionalized heterocycles via asym. tandem Staudinger/aza-Wittig/Ugi multicomponent reaction of azido(anhydro)-D-glucofuranoside or azido-D-ribofuranoside with acids and isocyanides)

RN 847740-12-9 CAPLUS

CN Spiro[cyclohexane-1,2'-[1,3]dioxolo[4,5-c]pyridine]-4'-carboxamide, 5'-benzoyl-N-cyclohexylhexahydro-7'-hydroxy-, (3'aS,4'R,7'R,7'aR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:546486 CAPLUS

DOCUMENT NUMBER: 141:106470

TITLE: Preparation of 5-chlorobenzimidazoles and related compounds as blood-coagulation factor Xa inhibitors.

INVENTOR(S): Priepke, Henning; Pfau, Roland; Gerlach, Kai; Gillard, James; Bauer, Eckhart; Wienen, Wolfgang; Handschuh, Sandra; Nar, Herbert

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. Kg, Germany; Dahmann, Georg

SOURCE: PCT Int. Appl., 502 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

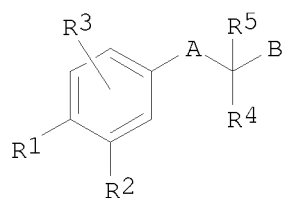
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 3

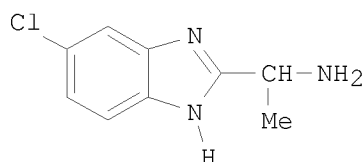
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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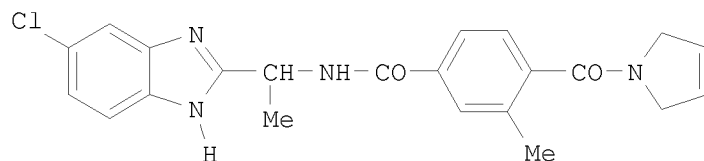
WO 2004056784	A1	20040708	WO 2003-EP14195	20031213
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10259407	A1	20040701	DE 2002-10259407	20021219
DE 10335545	A1	20050602	DE 2003-10335545	20030802
CA 2510846	A1	20040708	CA 2003-2510846	20031213
AU 2003292239	A1	20040714	AU 2003-292239	20031213
EP 1575925	A1	20050921	EP 2003-767800	20031213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006514987	T	20060518	JP 2005-502541	20031213
PRIORITY APPLN. INFO.:			DE 2002-10259407	A 20021219
			DE 2003-10335545	A 20030802
			WO 2003-EP14195	W 20031213
OTHER SOURCE(S):			MARPAT 141:106470	
GI				



I



II



III

AB Title compds. I [R1 = amino, alkylamino, cycloalkylamino, etc.; R2 = H, halo, alkyl, etc.; R3 = H, alkyl; R4 = H, alkenyl, alkynyl, etc.; R5 = H, alkyl; A = carbonylamino, aminocarbonyl, with provisos; B = (un)substituted benzimidazol, 4-azabenzimidazol, 1-azanaphthalene, etc.] and their formulations and pharmaceutically acceptable salts were prepared For example, coupling of 3-methyl-4-(2,5-dihydropyrrol-1-ylcarbonyl)benzoic acid and amine II, e.g., prepared from 4-chloro-o-phenylenediamine in 6-steps, afforded chlorobenzimidazole III. Compds. I were claimed useful as antithrombotic agents.

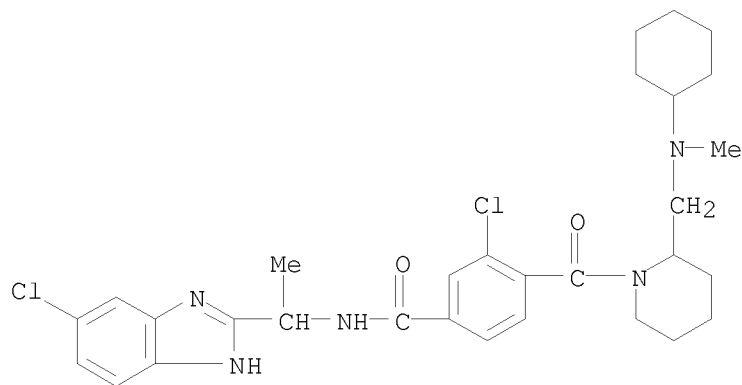
IT 719997-61-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 5-chlorobenzimidazoles and related compds. as blood-coagulation factor Xa inhibitors)

RN 719997-61-2 CAPLUS

CN Benzamide, 3-chloro-N-[1-(6-chloro-1H-benzimidazol-2-yl)ethyl]-4-[[2-[(cyclohexylmethylamino)methyl]-1-piperidiny]carbonyl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:412942 CAPLUS

DOCUMENT NUMBER: 140:406750

TITLE: Preparation of tetrahydroquinolines and tetrahydroisoquinolines as orexin receptor antagonists
INVENTOR(S): Branch, Clive Leslie; Pilleux, Jean-Pierre; Porter, Roderick Alan

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 25 pp.

CODEN: PIXXD2

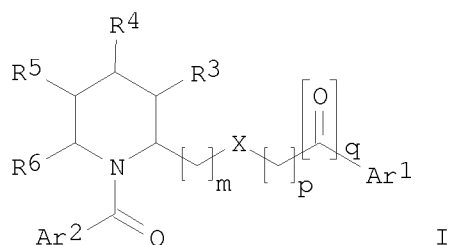
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041816	A1	20040521	WO 2003-EP12403	20031104
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			



AB The title azacyclic compds. I [R3 and R4 together with the carbons to which they are attached form (hetero)aromatic ring and R5 and R6 = H; or R4 and R5 together with the carbons to which they are attached form (hetero)aromatic ring and R3 and R6 = H; or R5 and R6 together with the carbons to which they are attached form (hetero)aromatic ring and R3 and R4 = H; m = 1-3; p = 0-1; q = 0-1 provided that when q = 1, p = 0; X = NR (R = H, alkyl); Ar1 = (un)substituted aryl, mono or bicyclic heteroaryl; Ar2 = (un)substituted bicyclic (hetero)aromatic ring], useful as orexin antagonists, were prepared Thus, reacting (5-bromopyrimidin-2-yl)-(1,2,3,4-tetrahydroisoquinolin-3-ylmethyl)amine (multi-step synthesis given) with 5-(4-fluorophenyl)-2-methylthiazole-4-carboxylic acid afforded 48% 1-{3-[(5-bromopyrimidin-2-ylamino)methyl]-3,4-dihydro-1H-isoquinolin-2-yl}-1-[5-(4-fluorophenyl)-2-methylthiazol-4-yl]methanone. The exemplified compds. I showed pKb values of >6.8 at the human cloned orexin-1 receptor, and pKb values of <7.0 at the human cloned orexin-2 receptor. The pharmaceutical composition comprising the compound I is claimed.

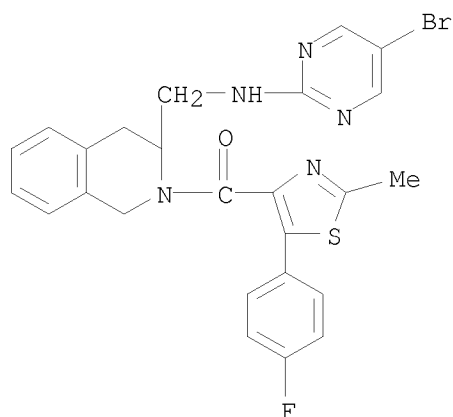
IT 690244-83-8P, 1-(3-((5-Bromopyrimidin-2-ylamino)methyl)-3,4-dihydro-1H-isoquinolin-2-yl)-1-(5-(4-fluorophenyl)-2-methylthiazol-4-yl)methanone 690244-84-9P, 1-(3-((5-Bromopyrimidin-2-ylamino)methyl)-3,4-dihydro-1H-isoquinolin-2-yl)-1-(4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl)methanone

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

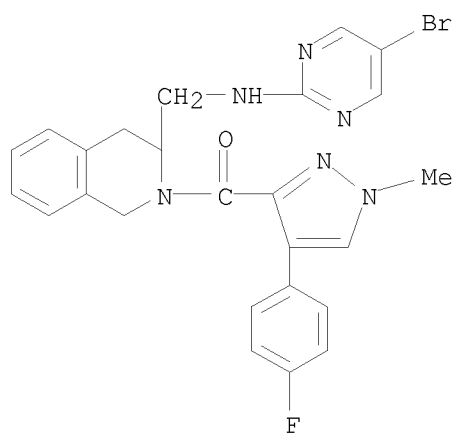
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(preparation of tetrahydroquinolines and tetrahydroisoquinolines as orexin
receptor antagonists)
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RN 690244-83-8 CAPLUS

CN Methanone, [3-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,4-dihydro-2 (1H)-isoquinolinyl] [5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)



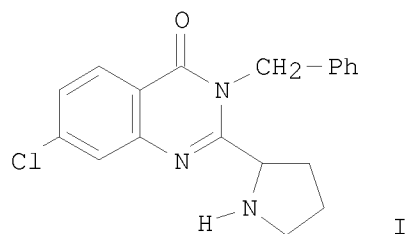
RN 690244-84-9 CAPLUS
 CN Methanone, [3-[[5-bromo-2-pyrimidinyl]amino]methyl]-3,4-dihydro-2(1H)-isoquinolinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (CA INDEX NAME)



L4 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:354730 CAPLUS
 DOCUMENT NUMBER: 140:350546
 TITLE: Heterocyclic-substituted quinazolinones preparation for treating cellular proliferative diseases
 INVENTOR(S): Bergnes, Gustave; Morgans, David J., Jr.
 PATENT ASSIGNEE(S): Cytokinetics, Inc., USA
 SOURCE: PCT Int. Appl., 61 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004034972	A2	20040429	WO 2003-US30788	20030930
WO 2004034972	A3	20041125		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003277079	A1	20040504	AU 2003-277079	20030930
EP 1558083	A2	20050803	EP 2003-808978	20030930
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2006501306	T	20060112	JP 2004-544787	20030930
US 20060264449	A1	20061123	US 2005-529745	20051114
PRIORITY APPLN. INFO.:			US 2002-414756P	P 20020930
			WO 2003-US30788	W 20030930
OTHER SOURCE(S):	MARPAT 140:350546			
GI				

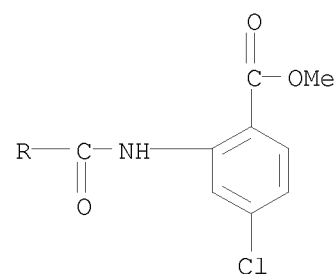
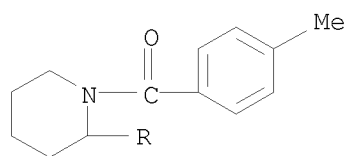


AB Heterocyclic-substituted quinazolinones were prepared for treating cellular proliferative diseases and disorders, for example, by modulating the activity of KSP. I and other similar compds. were prepared and examples were given, e.g., induction of mitotic arrest in cell populations treated with a KSP inhibitor, monopolar spindle formation following application of a KSP inhibitor, and inhibition of cellular proliferation in tumor cells lines with the inhibitors.

IT 681827-46-3P 681827-47-4P 681827-48-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (heterocyclic-substituted quinazolinones preparation for treating cellular proliferative diseases)

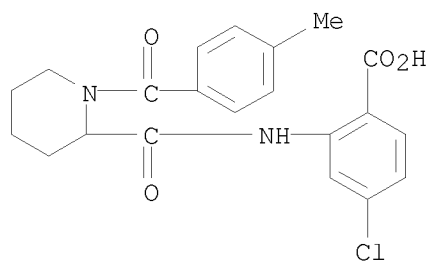
RN 681827-46-3 CAPLUS

CN Benzoic acid, 4-chloro-2-[[[1-(4-methylbenzoyl)-2-piperidinyl]carbonyl]amino]-, methyl ester (CA INDEX NAME)



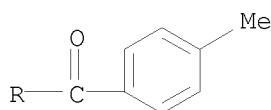
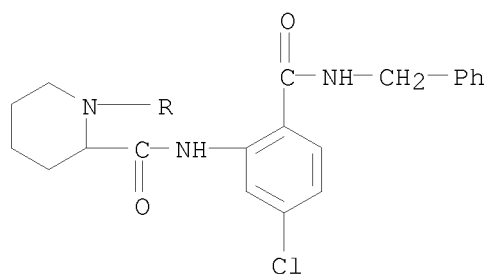
RN 681827-47-4 CAPLUS

CN Benzoic acid, 4-chloro-2-[[[1-(4-methylbenzoyl)-2-piperidinyl]carbonyl]amino]- (CA INDEX NAME)



RN 681827-48-5 CAPLUS

CN 2-Piperidinecarboxamide, N-[5-chloro-2-[(phenylmethyl)amino]carbonyl]phenyl]-1-(4-methylbenzoyl)- (CA INDEX NAME)

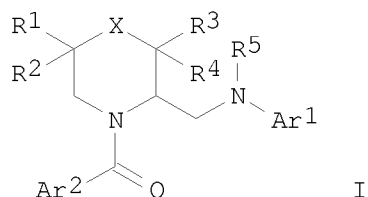


L4 ANSWER 16 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:267329 CAPLUS
 DOCUMENT NUMBER: 140:303688
 TITLE: Preparation of N-aroyl cyclic amines as orexin
 receptor antagonists
 INVENTOR(S): Branch, Clive Leslie; Coulton, Steven; Johns, Amanda;
 Nash, David John; Porter, Roderick Alan; Stemp,
 Geoffrey
 PATENT ASSIGNEE(S): Glaxo Group Limited, UK
 SOURCE: PCT Int. Appl., 35 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026866	A1	20040401	WO 2003-EP10412	20030917
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003262516	A1	20040408	AU 2003-262516	20030917
EP 1539747	A1	20050615	EP 2003-797310	20030917
EP 1539747	B1	20061102		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006504695	T	20060209	JP 2004-537127	20030917
AT 344261	T	20061115	AT 2003-797310	20030917
ES 2273083	T3	20070501	ES 2003-797310	20030917

US 20060040937 A1 20060223 US 2005-527833 20050816
 PRIORITY APPLN. INFO.: GB 2002-21690 A 20020918
 GB 2002-21691 A 20020918
 WO 2003-EP10412 W 20030917

OTHER SOURCE(S): MARPAT 140:303688
 GI



AB The title compds. [I; X = O, CR7R8, NH, a bond; R1, R2 are both H, or both are alkyl; or R1 and R2 together with the carbon to which they are attached form cycloalkyl or 4-6 membered heterocyclyl; R3, R4 are both H, or both are alkyl; or R3 and R4 together with the carbon to which they are attached form cycloalkyl or 4-6 membered heterocyclyl; R7, R8 are both H, or both are alkyl; or R7 and R8 together with the carbon to which they are attached form cycloalkyl or 4-6 membered heterocyclyl; R5 = H, alkyl, CO(alkyl); Ar1 = (un)substituted (hetero)aryl; Ar2 = (un)substituted Ph, 5-6 membered heterocyclyl, bicyclic (hetero)aryl; with the provisos], useful for treating or preventing diseases or disorders where an antagonist of a human orexin receptor is required, such as obesity and sleep disorders, were prepared Thus, reacting 5-(4-fluorophenyl)-2-methylthiazole-4-carbonyl chloride with (RS)-(5-bromopyrimidin-2-yl)(3,3-dimethylpiperidin-2-ylmethyl)amine (preparation given) in the presence of Et3N in CH2Cl2 afforded 78% (RS)-I [X = CH2; R1, R2 = H; R3, R4 = Me; R5 = H; Ar1 = 5-bromopyrimidin-2-yl; Ar2 = 5-(4-fluorophenyl)-2-methylthiazol-4-yl]. The exemplified compds. I showed pKb values in the range 7.0 to 9.7 at the human cloned orexin-1 receptor, and pKb values in the range <6.3 to 8.2 at the human cloned orexin-2 receptor. The pharmaceutical composition comprising the compound I is claimed.

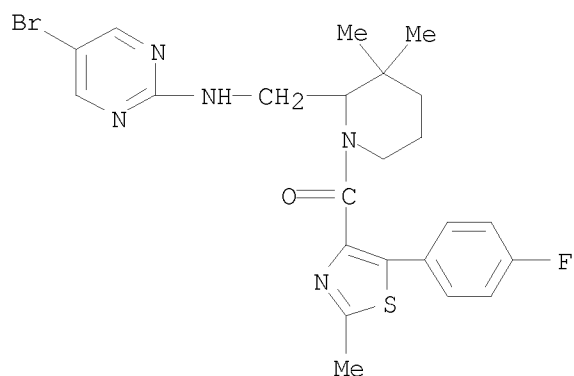
IT 676354-85-1P 676354-87-3P 676354-89-5P
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 676355-03-6P 676355-05-8P 676355-07-0P
 676355-09-2P 676355-11-6P 676355-13-8P
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 676355-51-4P 676355-54-7P 676355-56-9P
 676355-58-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-aroyle cyclic amines as orexin receptor antagonists for treating obesity and sleep disorders)

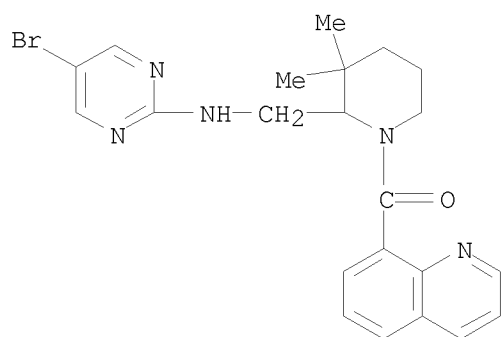
RN 676354-85-1 CAPLUS

CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)



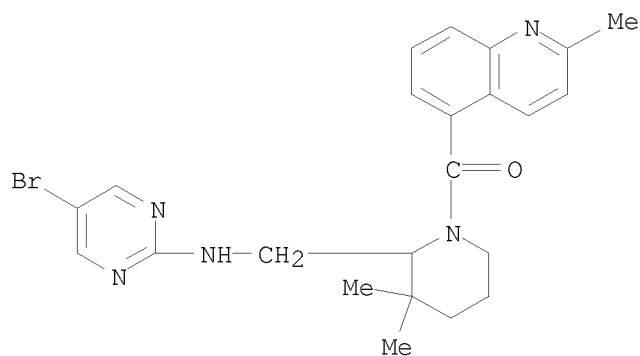
RN 676354-87-3 CAPLUS

CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl]-8-quinolinyl- (CA INDEX NAME)

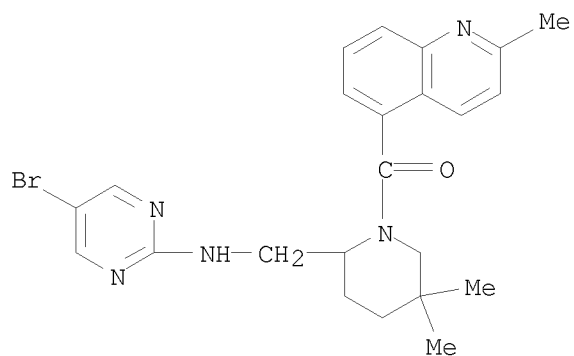


RN 676354-89-5 CAPLUS

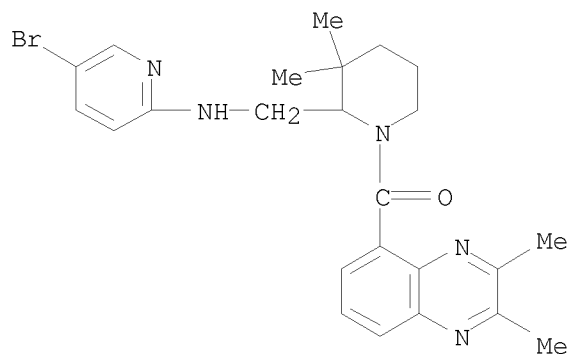
CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl](2-methyl-5-quinolinyl)- (CA INDEX NAME)



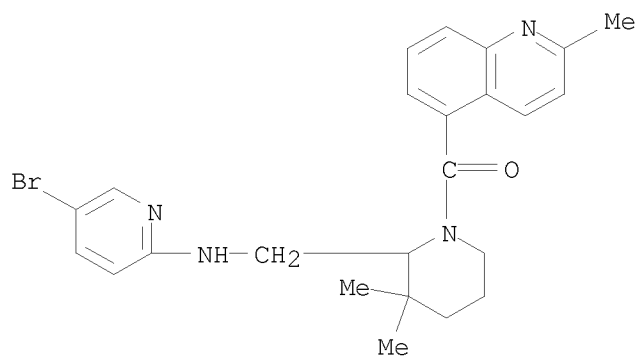
RN 676354-91-9 CAPLUS
 CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-5,5-dimethyl-1-piperidinyl](2-methyl-5-quinolinyl)- (CA INDEX NAME)



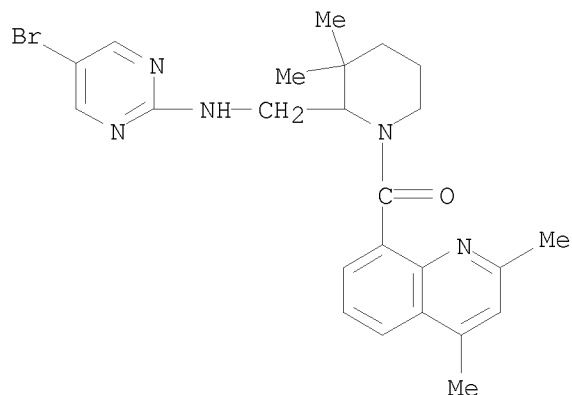
RN 676354-93-1 CAPLUS
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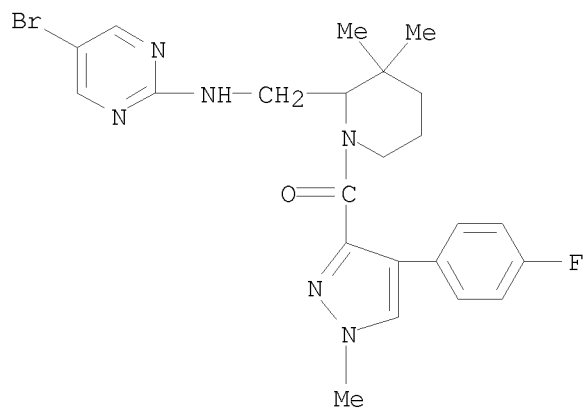
RN 676354-95-3 CAPLUS
 CN Methanone, [2-[[(5-bromo-2-pyridinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl](2-methyl-5-quinolinyl)- (CA INDEX NAME)



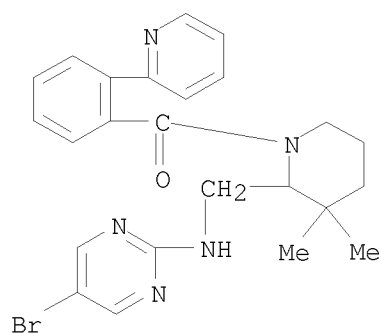
RN 676354-97-5 CAPLUS
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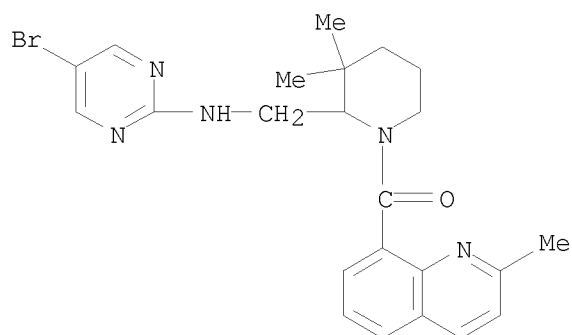
RN 676354-99-7 CAPLUS
 CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (CA INDEX NAME)



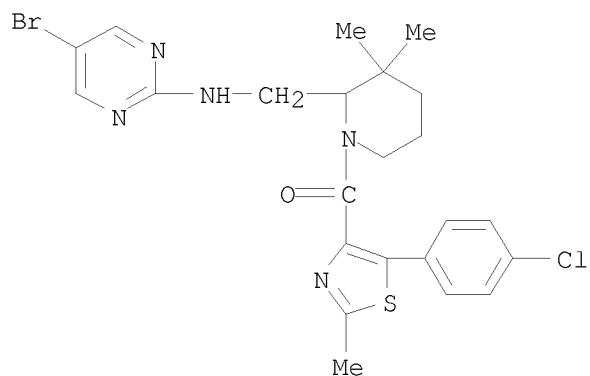
RN 676355-01-4 CAPLUS
 CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl][2-(2-pyridinyl)phenyl]- (CA INDEX NAME)



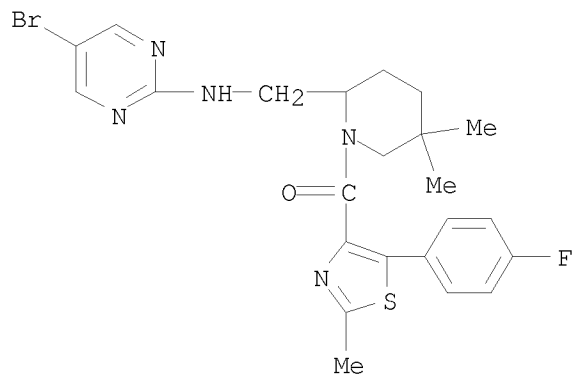
RN 676355-03-6 CAPLUS
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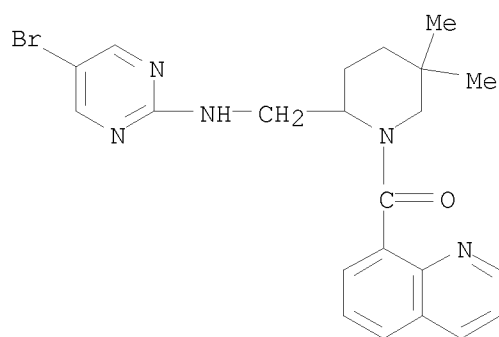
RN 676355-05-8 CAPLUS
 CN Methanone, [2-[[5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl]-5-(4-chlorophenyl)-2-methyl-4-thiazolyl)- (CA INDEX NAME)



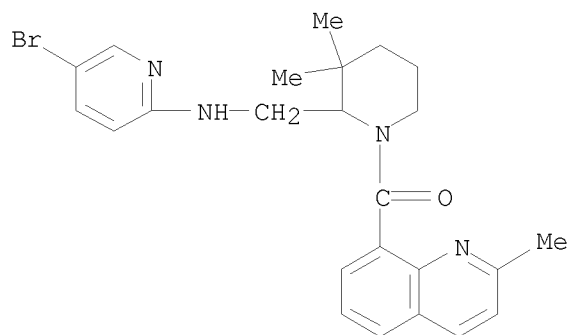
RN 676355-07-0 CAPLUS
 CN Methanone, [2-[[5-bromo-2-pyrimidinyl)amino]methyl]-5,5-dimethyl-1-piperidinyl]-5-(4-fluorophenyl)-2-methyl-4-thiazolyl)- (CA INDEX NAME)



RN 676355-09-2 CAPLUS
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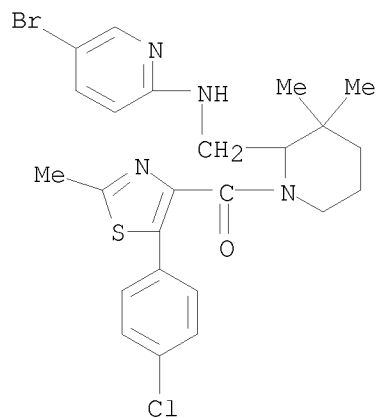


RN 676355-11-6 CAPLUS
 CN Methanone, [2-[(5-bromo-2-pyridinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl](2-methyl-8-quinolinyl)- (CA INDEX NAME)



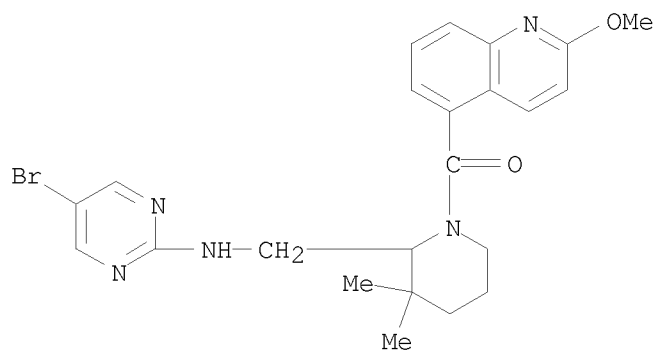
RN 676355-13-8 CAPLUS
 CN Methanone, [2-[(5-bromo-2-pyridinyl)amino]methyl]-3,3-dimethyl-1-

piperidinyl][5-(4-chlorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)



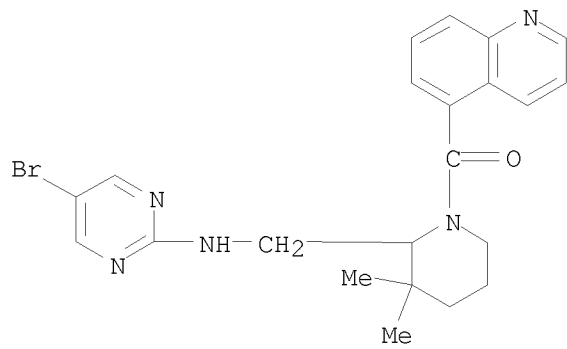
RN 676355-15-0 CAPLUS

CN Methanone, [2-[[5-(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl](2-methoxy-5-quinolinyl)- (CA INDEX NAME)



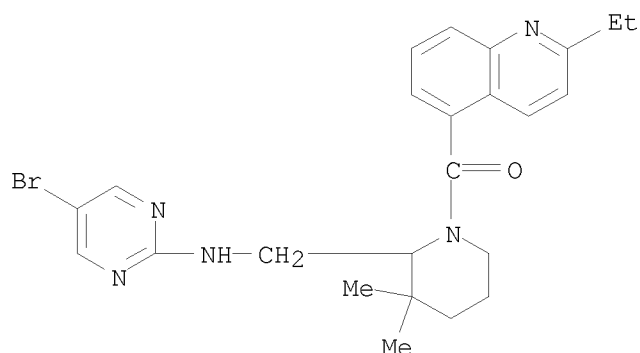
RN 676355-17-2 CAPLUS

CN Methanone, [2-[[5-(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl]-5-quinolinyl- (CA INDEX NAME)



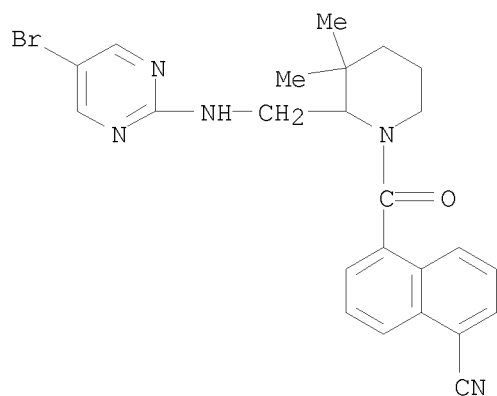
RN 676355-19-4 CAPLUS

CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl](2-ethyl-5-quinolinyl)- (CA INDEX NAME)



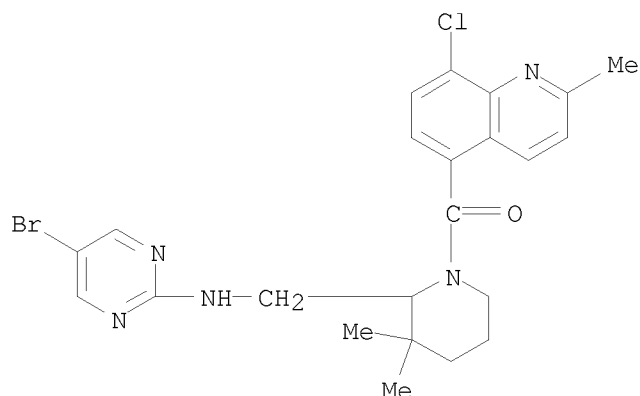
RN 676355-21-8 CAPLUS

CN 1-Naphthalenecarbonitrile, 5-[[2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl]carbonyl]- (CA INDEX NAME)



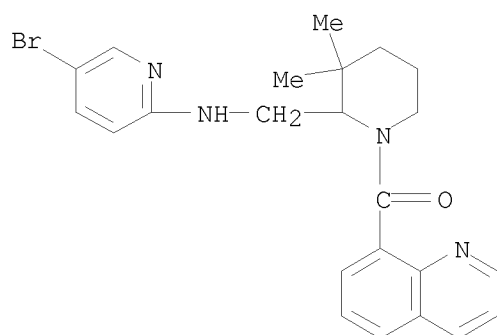
RN 676355-23-0 CAPLUS

CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl](8-chloro-2-methyl-5-quinolinyl)- (CA INDEX NAME)



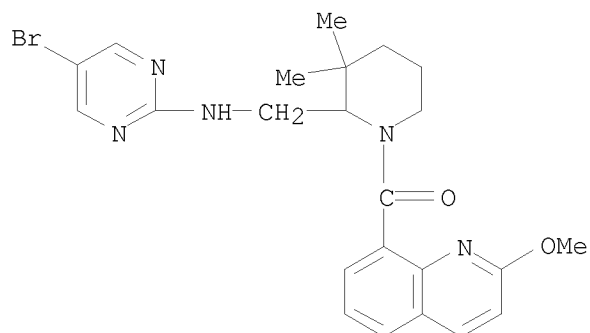
RN 676355-25-2 CAPLUS

CN Methanone, [2-[[5-bromo-2-pyridinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl]-8-quinolinyl- (CA INDEX NAME)



RN 676355-27-4 CAPLUS

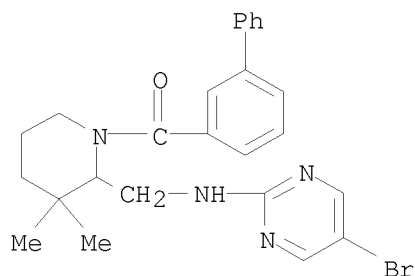
CN Methanone, [2-[[5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl](2-methoxy-8-quinolinyl)- (CA INDEX NAME)



RN 676355-29-6 CAPLUS

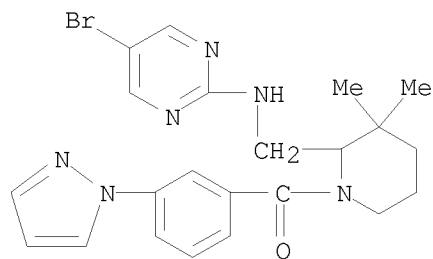
CN Methanone, [1,1'-biphenyl]-3-yl[2-[[5-bromo-2-pyrimidinyl)amino]methyl]-

3,3-dimethyl-1-piperidinyl]- (CA INDEX NAME)



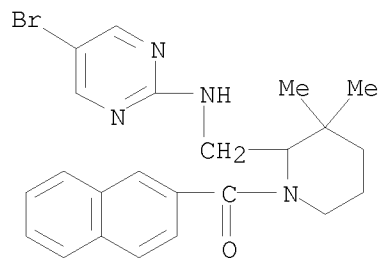
RN 676355-31-0 CAPLUS

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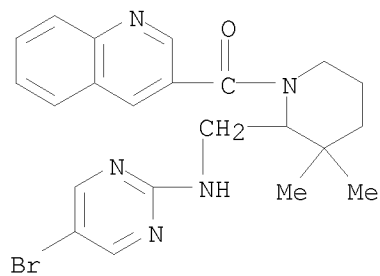
RN 676355-33-2 CAPLUS

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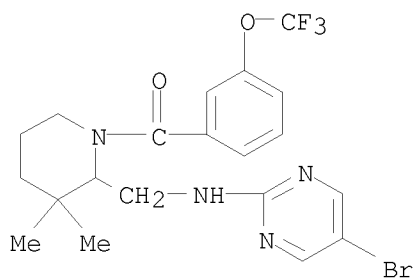


RN 676355-35-4 CAPLUS

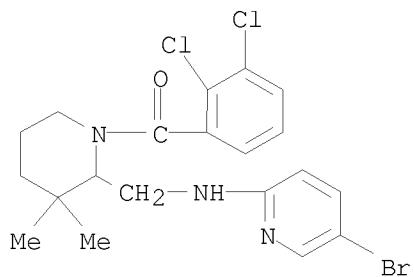
CN Methanone, [2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl]-3-quinoliny]- (CA INDEX NAME)



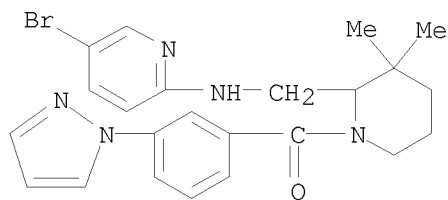
RN 676355-37-6 CAPLUS
 CN Methanone, [2-[[5-bromo-2-pyrimidinyl]amino]methyl]-3,3-dimethyl-1-piperidinyll[3-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



RN 676355-39-8 CAPLUS
 CN Methanone, [2-[[5-bromo-2-pyridinyl]amino]methyl]-3,3-dimethyl-1-piperidinyll(2,3-dichlorophenyl)- (CA INDEX NAME)

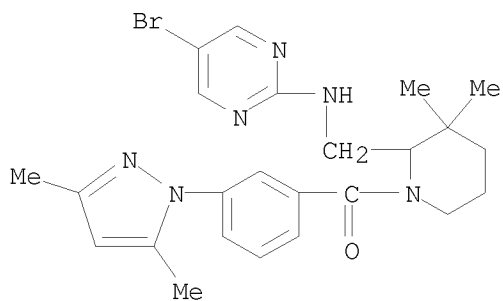


RN 676355-41-2 CAPLUS
 CN Methanone, [2-[[5-bromo-2-pyridinyl]amino]methyl]-3,3-dimethyl-1-piperidinyll[3-(1H-pyrazol-1-yl)phenyl]- (CA INDEX NAME)



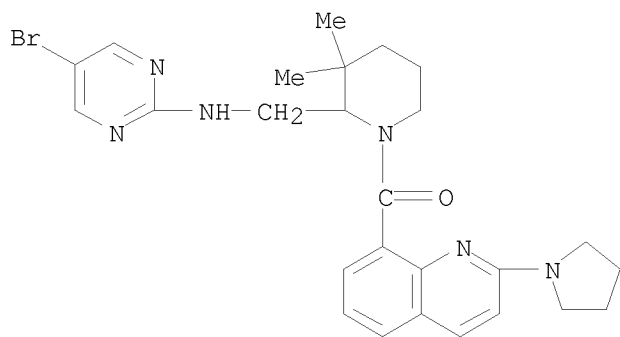
RN 676355-43-4 CAPLUS

CN Methanone, [2-[[5-bromo-2-pyrimidinyl]amino]methyl]-3,3-dimethyl-1-piperidinyl][3-(3,5-dimethyl-1H-pyrazol-1-yl)phenyl]- (CA INDEX NAME)



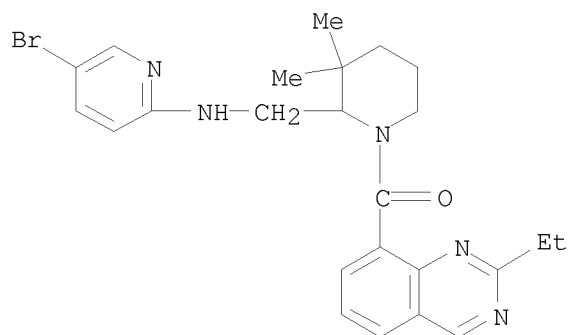
RN 676355-45-6 CAPLUS

CN Methanone, [2-[[5-bromo-2-pyrimidinyl]amino]methyl]-3,3-dimethyl-1-piperidinyl][2-(1-pyrrolidinyl)-8-quinolinyl]- (CA INDEX NAME)

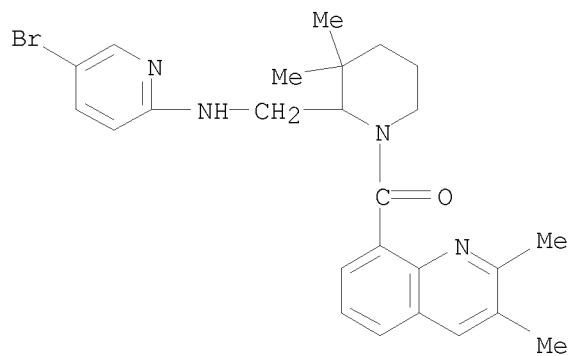


RN 676355-47-8 CAPLUS

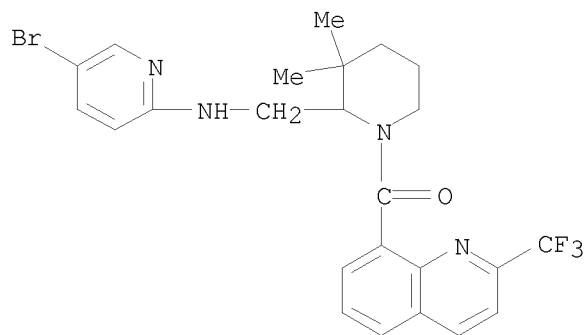
CN Methanone, [2-[[5-bromo-2-pyridinyl]amino]methyl]-3,3-dimethyl-1-piperidinyl](2-ethyl-8-quinazolinyl)- (CA INDEX NAME)



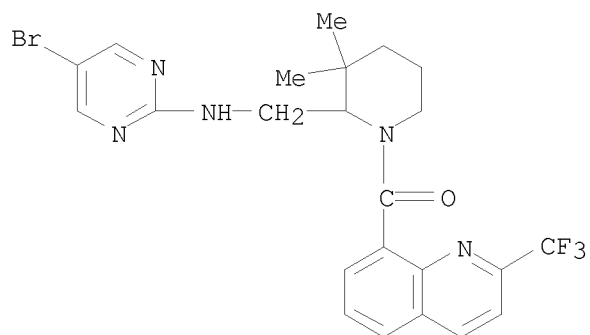
RN 676355-49-0 CAPLUS
 CN Methanone, [2-[[(5-bromo-2-pyridinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl] (2,3-dimethyl-8-quinolinyl)- (CA INDEX NAME)



RN 676355-51-4 CAPLUS
 CN Methanone, [2-[[(5-bromo-2-pyridinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl] [2-(trifluoromethyl)-8-quinolinyl]- (CA INDEX NAME)

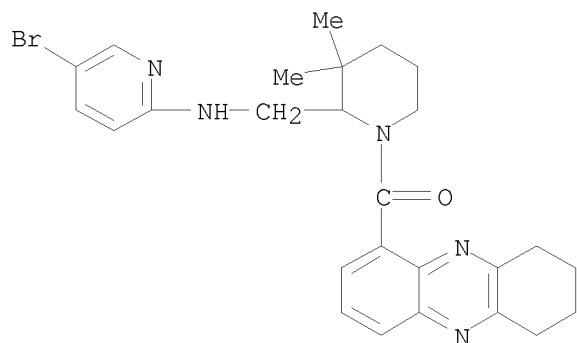


RN 676355-54-7 CAPLUS
 CN Methanone, [2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidinyl] [2-(trifluoromethyl)-8-quinolinyl]- (CA INDEX NAME)



RN 676355-56-9 CAPLUS

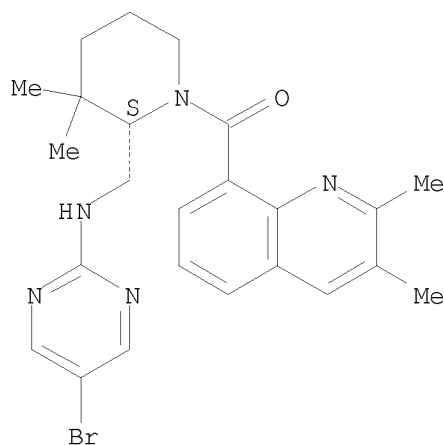
CN Methanone, [2-[(5-bromo-2-pyridinyl)amino]methyl]-3,3-dimethyl-1-piperidiny] (6,7,8,9-tetrahydro-1-phenazinyl)- (CA INDEX NAME)



RN 676355-58-1 CAPLUS

CN Methanone, [(2S)-2-[(5-bromo-2-pyrimidinyl)amino]methyl]-3,3-dimethyl-1-piperidiny] (2,3-dimethyl-8-quinolinyl)- (CA INDEX NAME)

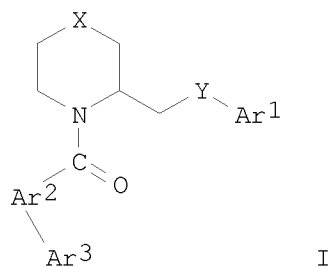
Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:491048 CAPLUS
 DOCUMENT NUMBER: 139:69283
 TITLE: Preparation of N-aroyle cyclic amine derivatives as orexin receptor antagonists
 INVENTOR(S): Branch, Clive Leslie; Nash, David John; Stemp, Geoffrey
 PATENT ASSIGNEE(S): Smithkline Beecham PLC, UK
 SOURCE: PCT Int. Appl., 50136 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051368	A1	20030626	WO 2002-GB5773	20021218
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002352447	A1	20030630	AU 2002-352447	20021218
PRIORITY APPLN. INFO.:			GB 2001-30335	A 20011219
			WO 2002-GB5773	W 20021218
OTHER SOURCE(S):			MARPAT 139:69283	
GI				



AB N-aroyle cyclic amine derivs. [I; Ar1 = (un)substituted Ph, naphthyl, 5- or 6-membered or bicyclic heteroaryl containing ≤3 N, O, S atoms; Ar2 = (un)substituted Ph, 5- or 6-membered heteroaryl containing ≤3 N, O, S atoms; Ar3 = RC6H4; R = O(CH2)mNR1R2, (CH2)mNR1R2; R1, R2 = H,

(un)substituted C1-6 alkyl; R1R2N can form (C3-6)azacycloalkane or (C3-6) (2-oxo)azacycloalkane ring, etc.; X = bond, O, NR3, (CH2)n; R3 = H, (un)substituted C1-6 alkyl; Y = (CH2)qNHC(O), (CH2)qCH:CH(CH2)p, etc.; m = 2-6; n, q = 1, 2; p = 0, 1] or their pharmaceutically acceptable salts, nonpeptide antagonists of human orexin receptors, useful for the treatment of diseases or disorders where an antagonist of a human orexin receptor is required, were prepared. For example, adding 0.088 g 2-[3-(2-dimethylaminoethoxy)phenyl]thiophene-3-carboxylic acid (preparation given) to 0.126 g (S)-2-(3,4-difluorobenzamidomethyl)piperidine (preparation given) in 4 mL CH2Cl2 at ambient temperature followed by 0.076 g

1-(3-dimethylaminopropyl)-3-

Et carbodiimide-HCl and 0.01 g 1-hydroxybenzotriazole and shaking the mixture for 18 h gave 0.079 g (S)-2-(3,4-difluorobenzamidomethyl)-1-[[3-[2-[3-(2-dimethylaminoethoxy)phenyl]]thiophenyl]carbonyl]piperidine. The exemplified compds. I showed pKb values >7.1-8.4 at the human cloned orexin-1 receptor, and pKb values 6.8-8.4 at the human cloned orexin-2 receptor.

IT 475103-93-6P 549526-48-9P

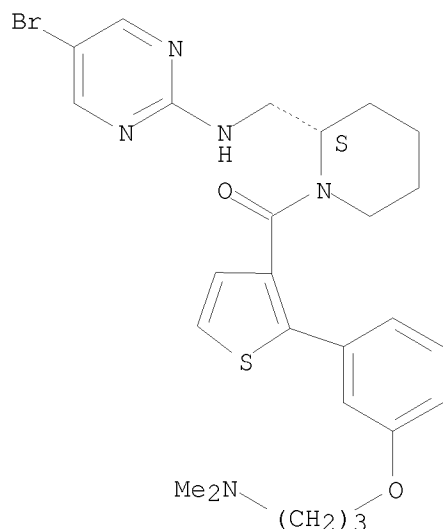
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of N-aroyl cyclic amine derivs. as orexin receptor antagonists)

RN 475103-93-6 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][2-[3-[3-(dimethylamino)propoxy]phenyl]-3-thienyl]- (CA INDEX NAME)

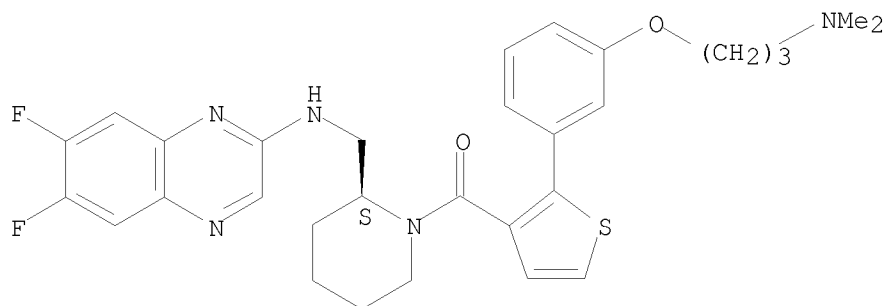
Absolute stereochemistry.



RN 549526-48-9 CAPLUS

CN Methanone, [(2S)-2-[[[(6,7-difluoro-2-quinoxaliny)amino]methyl]-1-piperidinyl][2-[3-[3-(dimethylamino)propoxy]phenyl]-3-thienyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:356201 CAPLUS

DOCUMENT NUMBER: 138:368888

TITLE: Pyrazolecarboxamides and -sulfonamides as sodium channel blockers

INVENTOR(S): Atkinson, Robert Nelson; Gross, Michael Francis

PATENT ASSIGNEE(S): Icagen, Inc., USA

SOURCE: PCT Int. Appl., 132 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

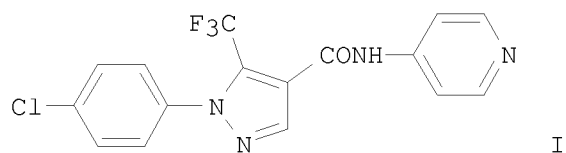
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003037274	A2	20030508	WO 2002-US35172	20021101
WO 2003037274	A3	20031030		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2465207	A1	20030508	CA 2002-2465207	20021101
AU 2002363250	A1	20030512	AU 2002-363250	20021101
EP 1451160	A2	20040901	EP 2002-799175	20021101
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
US 20050049237	A1	20050303	US 2002-286304	20021101
US 7223782	B2	20070529		
US 20080064690	A1	20080313	US 2007-740845	20070426
PRIORITY APPLN. INFO.:			US 2001-335958P	P 20011101
			US 2002-286304	A1 20021101
			WO 2002-US35172	W 20021101

OTHER SOURCE(S): MARPAT 138:368888

GI



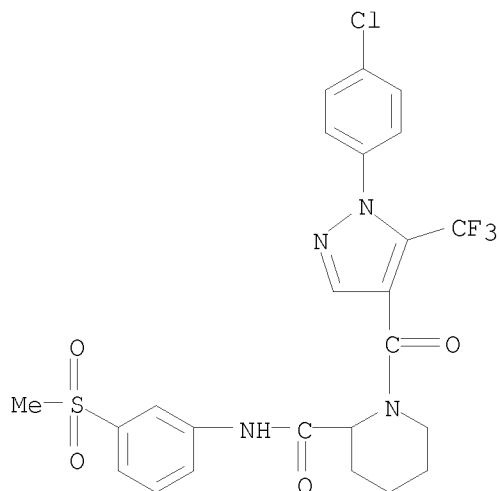
AB Pyrazolecarboxamides and -sulfonamides were prepared for use in the treatment of diseases through the inhibition of sodium ion flux through voltage-dependent sodium channels, especially pain and chronic pain. Thus, the amide I was prepared by amidation of the acid chloride with the amine and showed activity at the PN3 Na channel in the 4.1-10 μ M range.

IT 521933-67-5P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolecarboxamides and -sulfonamides as sodium channel blockers)

RN 521933-67-5 CAPLUS

CN 2-Piperidinecarboxamide, 1-[[1-(4-chlorophenyl)-5-(trifluoromethyl)-1H-pyrazol-4-yl]carbonyl]-N-[3-(methylsulfonyl)phenyl]- (CA INDEX NAME)



L4 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:888706 CAPLUS

DOCUMENT NUMBER: 137:370363

TITLE: Preparation of 4-amino-azepan-3-one derivatives as protease inhibitors

INVENTOR(S): Xie, Ren; Yamashita, Dennis S.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 37 pp.

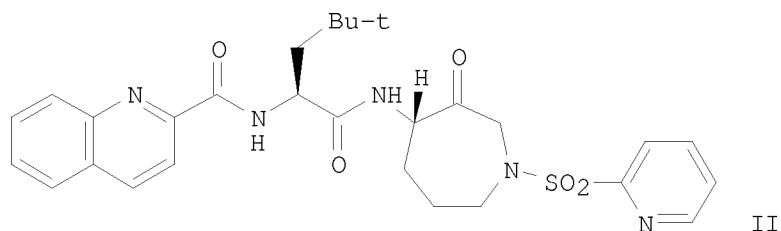
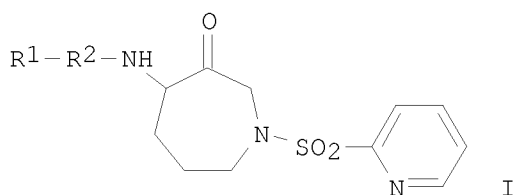
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092563	A2	20021121	WO 2002-US15376	20020515
WO 2002092563	A3	20030403		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002342682	A1	20021125	AU 2002-342682	20020515
EP 1401453	A2	20040331	EP 2002-744152	20020515
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004527575	T	20040909	JP 2002-589449	20020515
US 20040157828	A1	20040812	US 2003-478619	20031117
PRIORITY APPLN. INFO.:			US 2001-291545P	P 20010517
			US 2001-292646P	P 20010522
			WO 2002-US15376	W 20020515
OTHER SOURCE(S):			MARPAT 137:370363	
GI				



AB 4-Aminoazepan-3-one derivs. of formula I [R₁ = 3-methylbenzofuran-2-carbonyl, benzofuran-2-carbonyl, 5-methoxybenzofuran-2-carbonyl, benzothiophene-2-carbonyl, quinoline-2-carbonyl, quinoline-3-carbonyl, thiophene-2-carbonyl, thiophene-3-carbonyl, 5-methylthiophene-2-carbonyl, furan-2-carbonyl, furan-3-carbonyl, thieno[3,2-b]thiophene-2-carbonyl; R₂ = L-tert-butylalaninyl, L-2-thiophenylalaninyl, L-cyclohexylglycinyl, L-allo-isoleucinyl, tetrahydroisoquinoline-3-carbonyl, L-prolinyl, (S)-2-amino-4-methanesulfonylbutanoyl, (S)-piperidine-2-carbonyl] are

prepared which inhibit proteases, including cathepsin K. The compds. are useful for treating diseases of excessive bone loss or cartilage or matrix degradation, including osteoporosis, gingival disease including gingivitis and periodontitis, arthritis, more specifically, osteoarthritis and rheumatoid arthritis, Paget's disease, hypercalcemia of malignancy, and metabolic bone disease. Thus, II was prepared from 4-amino-3-hydroxyazepane-1-carboxylic acid benzyl ester hydrochloride, 2-pyridinesulfonyl chloride, Boc-L-tert-butylalanine and quinaldic acid. The prepared compds. had Ki values between 2 nM and 1000 nM against cathepsin K in inhibition assays.

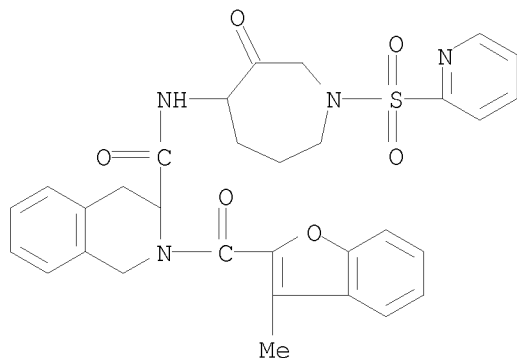
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475286-56-7P 475286-57-8P 475286-58-9P
475286-59-0P 475286-60-3P 475286-61-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminoazepanone derivs. as protease inhibitors)

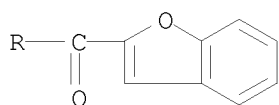
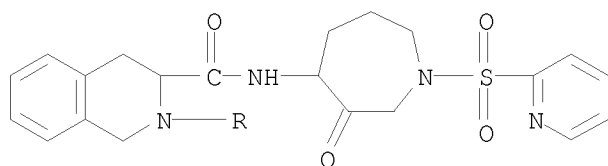
RN 475286-20-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro-2-[(3-methyl-2-benzofuranyl)carbonyl]- (CA INDEX NAME)

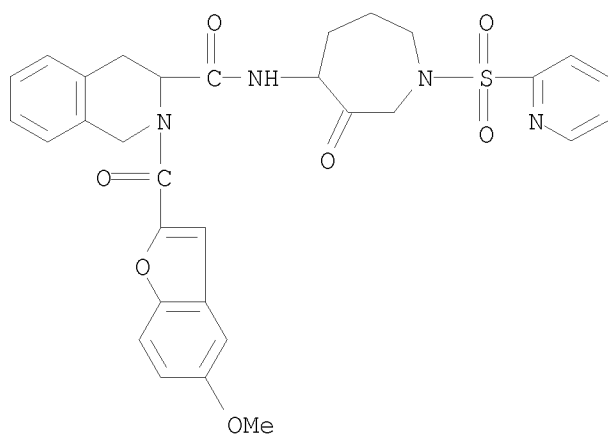


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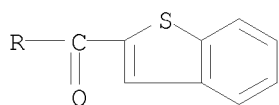
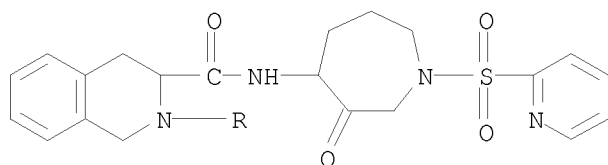
CN 3-Isoquinolinecarboxamide, 2-(2-benzofuranylcabonyl)-N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



RN 475286-22-7 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro-2-[(5-methoxy-2-benzofuranyl)carbonyl]- (CA INDEX NAME)

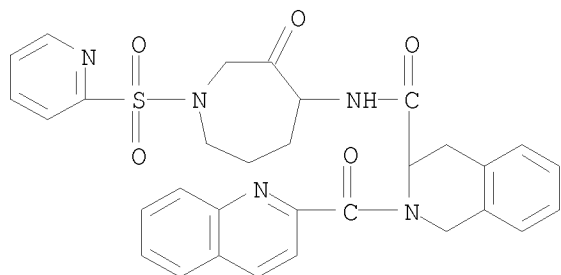


RN 475286-23-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-(benzo[b]thien-2-ylcarbonyl)-N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



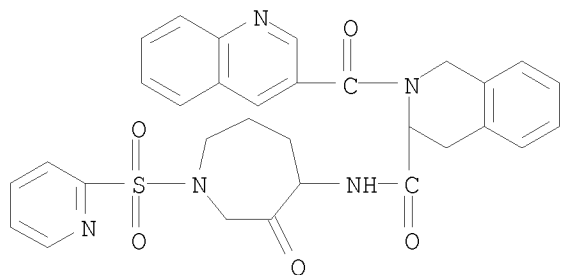
RN 475286-24-9 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro-2-(2-quinolinylcarbonyl)- (CA INDEX NAME)



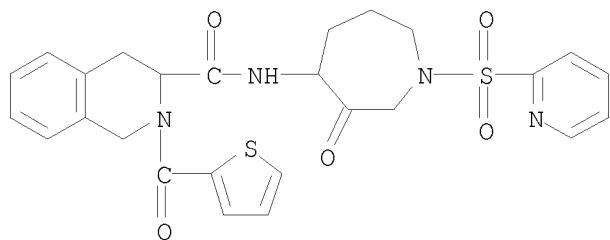
RN 475286-25-0 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro-2-(3-quinolinylcarbonyl)- (CA INDEX NAME)



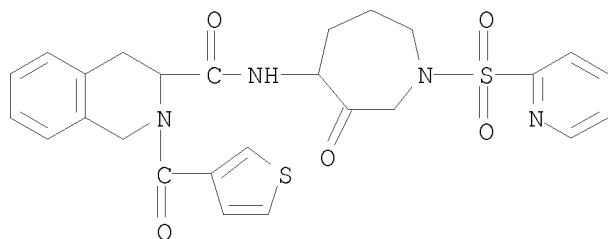
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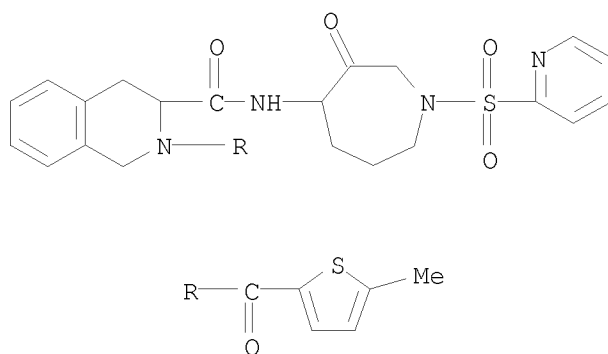
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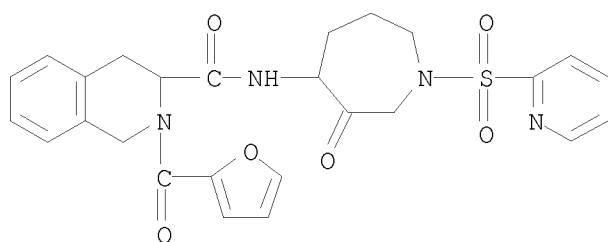
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CN 3-Isoquinolinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro-2-[(5-methyl-2-thienyl)carbonyl]- (CA INDEX NAME)



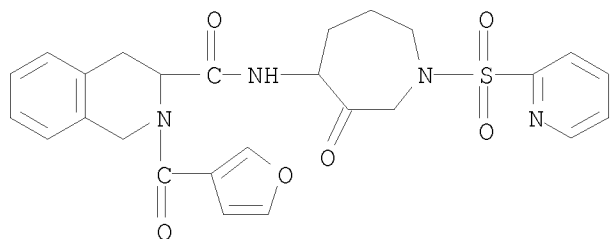
RN 475286-29-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(2-furanylcarbonyl)-N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



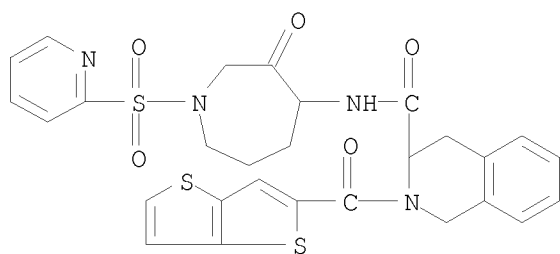
RN 475286-30-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-furanylcarbonyl)-N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



RN 475286-31-8 CAPLUS

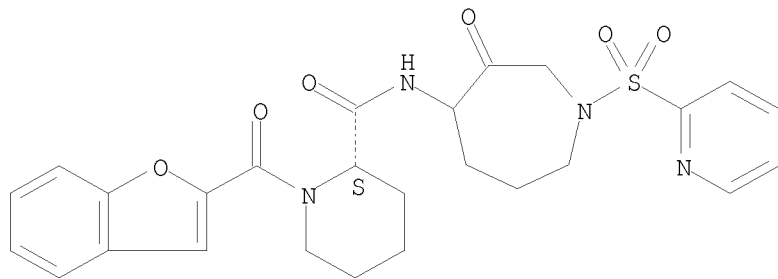
CN 3-Isoquinolinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1,2,3,4-tetrahydro-2-(thieno[3,2-b]thien-2-ylcarbonyl)- (CA INDEX NAME)



RN 475286-56-7 CAPLUS

CN 2-Piperidinecarboxamide, 1-(2-benzofuranylcarbonyl)-N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-, (2S)- (CA INDEX NAME)

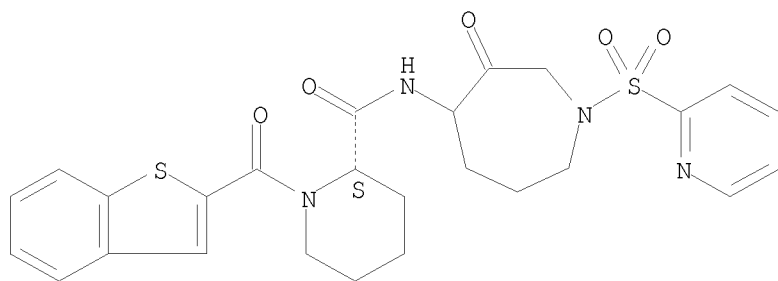
Absolute stereochemistry.



RN 475286-57-8 CAPLUS

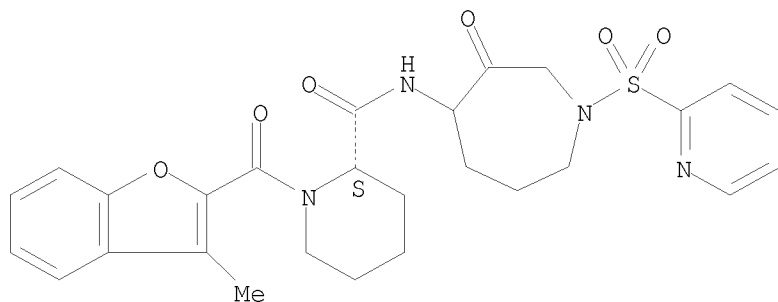
CN 2-Piperidinecarboxamide, 1-(benzo[b]thien-2-ylcarbonyl)-N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



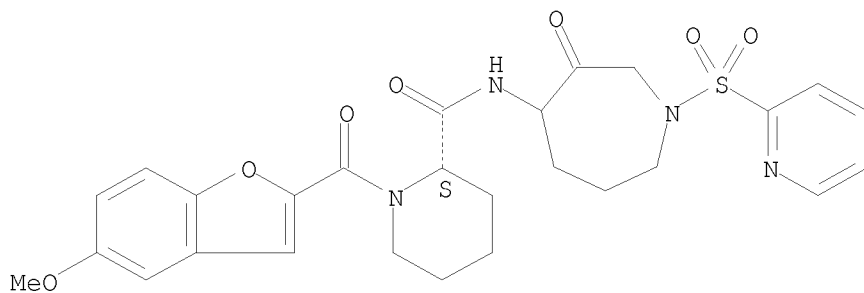
RN 475286-58-9 CAPLUS
 CN 2-Piperidinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1-[(3-methyl-2-benzofuranyl)carbonyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



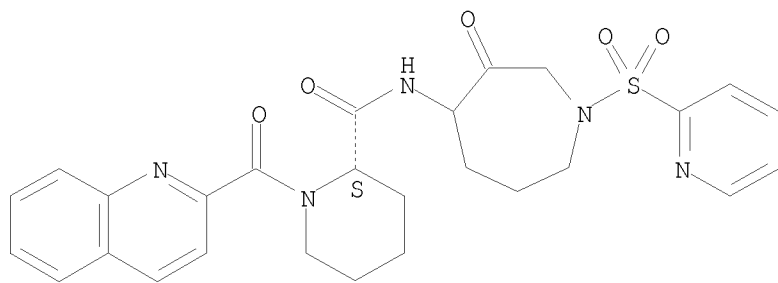
RN 475286-59-0 CAPLUS
 CN 2-Piperidinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1-[(5-methoxy-2-benzofuranyl)carbonyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 475286-60-3 CAPLUS
 CN 2-Piperidinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1-(2-quinolinylcarbonyl)-, (2S)- (CA INDEX NAME)

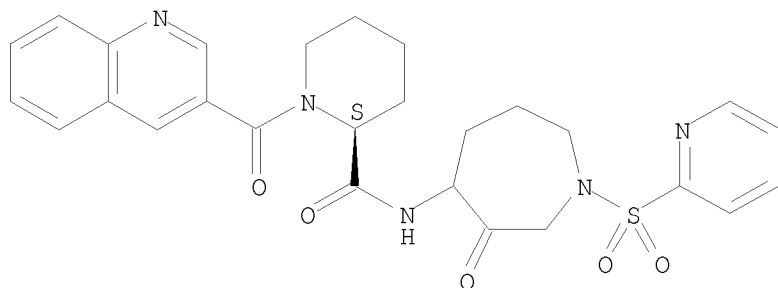
Absolute stereochemistry.



RN 475286-61-4 CAPLUS

CN 2-Piperidinecarboxamide, N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]-1-(3-quinolinylcarbonyl)-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:868931 CAPLUS

DOCUMENT NUMBER: 137:370109

TITLE: Preparation of N-aroyl cyclic amines as orexin antagonists

INVENTOR(S): Branch, Clive Leslie; Coulton, Steven; Johns, Amanda; Johnson, Christopher Norbert; Porter, Roderick Alan; Stemp, Geoffrey; Thewlis, Kevin

PATENT ASSIGNEE(S): Smithkline Beecham PLC, UK

SOURCE: PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

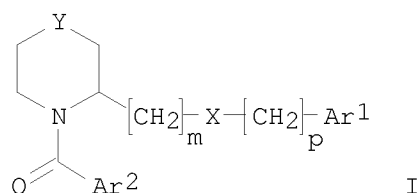
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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EP 1385845	B1	20080109		
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CN 1633433	A	20050629	CN 2002-811986	20020502
NZ 528851	A	20060331	NZ 2002-528851	20020502
AT 383359	T	20080115	AT 2002-722482	20020502
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			GB 2001-21303	A 20010903
			GB 2001-30331	A 20011219
			GB 2001-30392	A 20011219
			EP 2002-722482	A3 20020502
			WO 2002-GB2042	W 20020502
OTHER SOURCE(S):			MARPAT 137:370109	
GI				



AB The title compds. [I; Y = a bond, O, (CH₂)_n (wherein n = 1-3); m = 1-3; p = 0-1; X = NR (R = H, alkyl); Ar₁ = (un)substituted aryl, a mono or bicyclic heteroaryl containing up to 3 heteroatoms selected from N, O and S; Ar₂ = (un)substituted Ph, 5- or 6-membered heterocyclyl containing up to 3 heteroatoms selected from N, O and S; or Ar₂ = (un)substituted bicyclic aromatic or bicyclic heteroarom. group containing up to 3 heteroatoms selected from N, O and S; when Y = a bond, Ar₂ can not be 2-naphthyl; when Ar₁ = aryl, p is not 1], useful as antagonists of human orexin receptors, in particular orexin-1-receptors, were prepared. Thus, amidation of 2-(benzoxazol-2-ylaminomethyl)piperidine (preparation given) with

2-methyl-5-phenylthiazole-4-carbonyl chloride in CH₂Cl₂ afforded I [Y = CH₂; m = 1; p = 0; X = NH; Ar₁ = benzoxazol-2-yl; Ar₂ = 2-methyl-5-phenylthiazol-4-yl]. Exemplified compds. I showed pK_b of 6.7-9.7 at the human cloned orexin-1 receptor, and pK_b of 6.3-9.1 at the human cloned orexin-2 receptor.

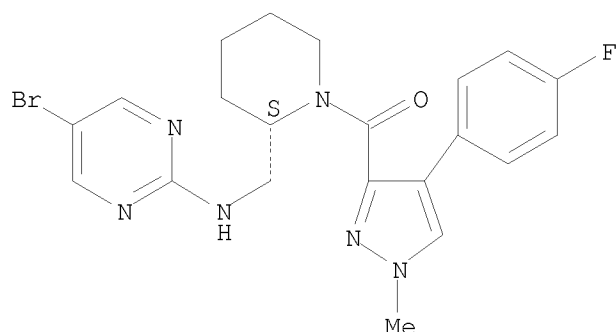
IT 475104-08-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of N-aroyl cyclic amines as orexin antagonists)

RN 475104-08-6 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 475102-53-5P 475102-54-6P 475102-55-7P
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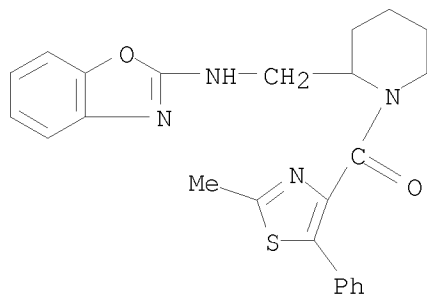
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of N-aroyl cyclic amines as orexin antagonists)

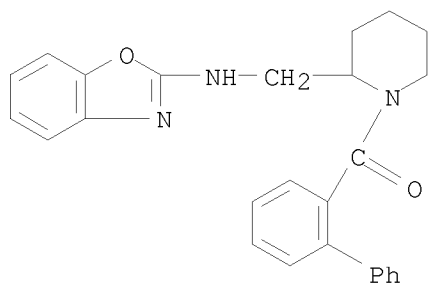
RN 475102-53-5 CAPLUS

CN Methanone, [2-[(2-benzoxazolylamino)methyl]-1-piperidinyl](2-methyl-5-
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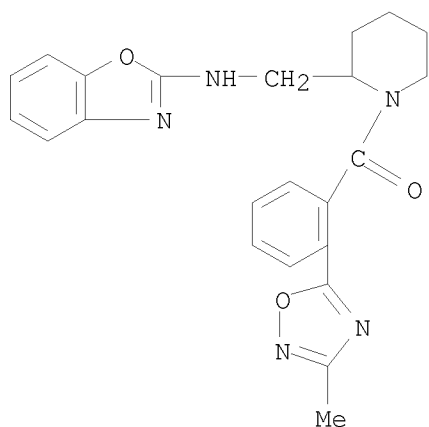
RN 475102-54-6 CAPLUS

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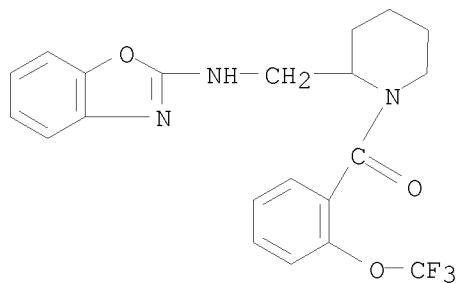
RN 475102-55-7 CAPLUS

CN Methanone, [2-[(2-benzoxazolylamino)methyl]-1-piperidinyl][2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]- (CA INDEX NAME)



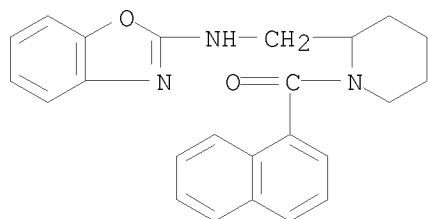
RN 475102-56-8 CAPLUS

CN Methanone, [2-[(2-benzoxazolylamino)methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

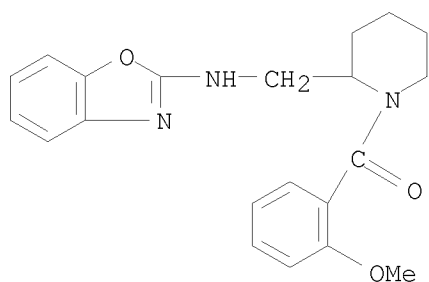


RN 475102-57-9 CAPLUS

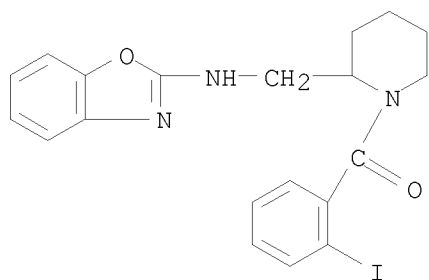
CN Methanone, [2-[(2-benzoxazolylamino)methyl]-1-piperidinyl]-1-naphthalenyl- (CA INDEX NAME)



RN 475102-58-0 CAPLUS
 CN Methanone, [2-[(2-benzoxazolylamino)methyl]-1-piperidinyl](2-methoxyphenyl)- (CA INDEX NAME)

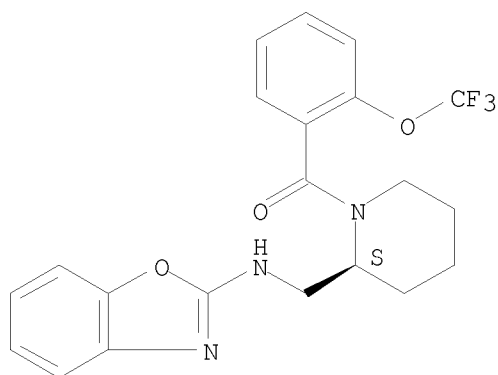


RN 475102-59-1 CAPLUS
 CN Methanone, [2-[(2-benzoxazolylamino)methyl]-1-piperidinyl](2-iodophenyl)- (CA INDEX NAME)



RN 475102-60-4 CAPLUS
 CN Methanone, [(2S)-2-[(2-benzoxazolylamino)methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

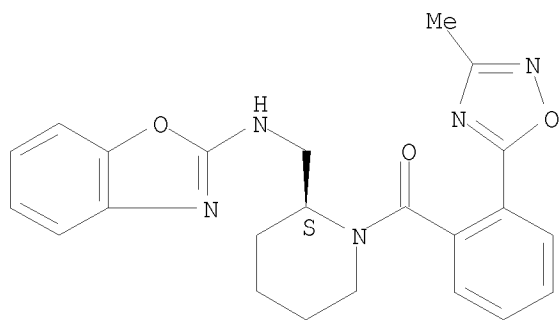
Absolute stereochemistry.



RN 475102-61-5 CAPLUS

CN Methanone, [(2S)-2-[(2-benzoxazolylamino)methyl]-1-piperidiny] [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]- (CA INDEX NAME)

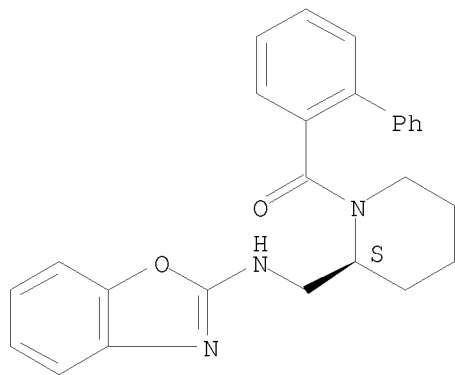
Absolute stereochemistry.



RN 475102-62-6 CAPLUS

CN Methanone, [(2S)-2-[(2-benzoxazolylamino)methyl]-1-piperidiny] [1,1'-biphenyl]-2-yl- (CA INDEX NAME)

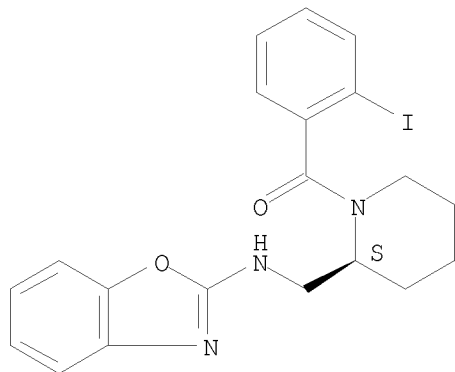
Absolute stereochemistry.



RN 475102-63-7 CAPLUS

CN Methanone, [(2S)-2-[(2-benzoxazolylamino)methyl]-1-piperidinyl](2-iodophenyl)- (CA INDEX NAME)

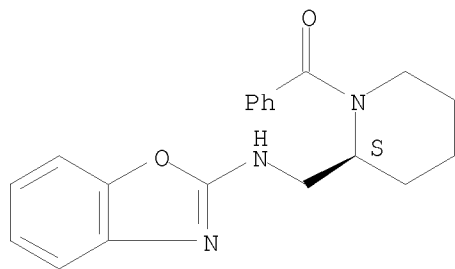
Absolute stereochemistry.



RN 475102-64-8 CAPLUS

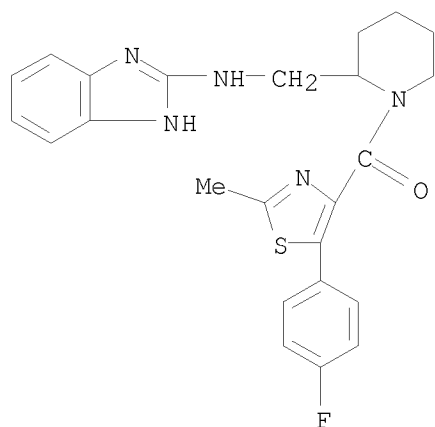
CN Methanone, [(2S)-2-[(2-benzoxazolylamino)methyl]-1-piperidinyl]phenyl- (CA INDEX NAME)

Absolute stereochemistry.



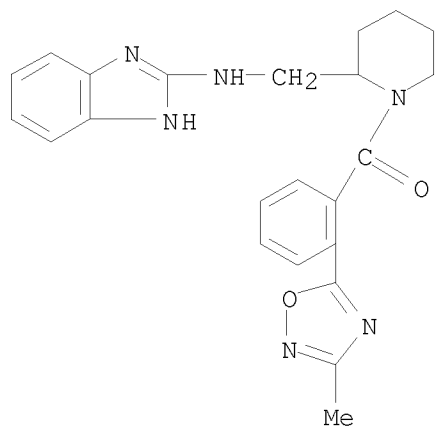
RN 475102-65-9 CAPLUS

CN Methanone, [2-[(1H-benzimidazol-2-ylamino)methyl]-1-piperidinyl][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)



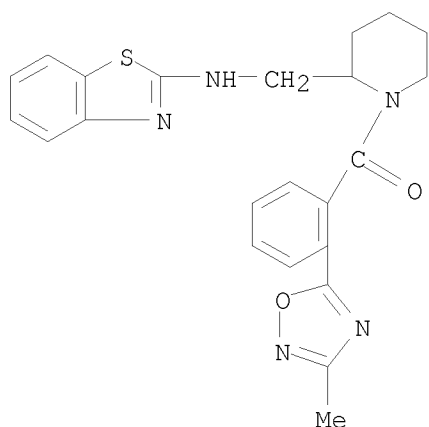
RN 475102-66-0 CAPLUS

CN Methanone, [2-[(1H-benzimidazol-2-ylamino)methyl]-1-piperidinyl][2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]- (CA INDEX NAME)



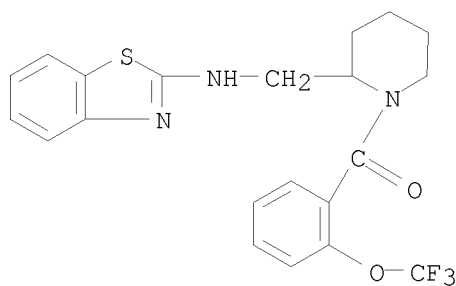
RN 475102-67-1 CAPLUS

CN Methanone, [2-[(2-benzothiazolylamino)methyl]-1-piperidinyl][2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]- (CA INDEX NAME)



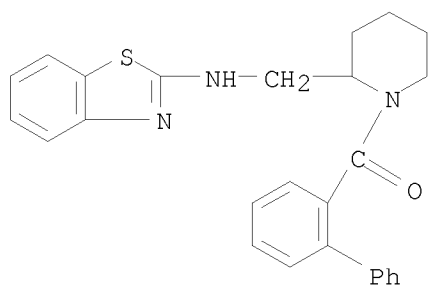
RN 475102-68-2 CAPLUS

CN Methanone, [2-[(2-benzothiazolylamino)methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



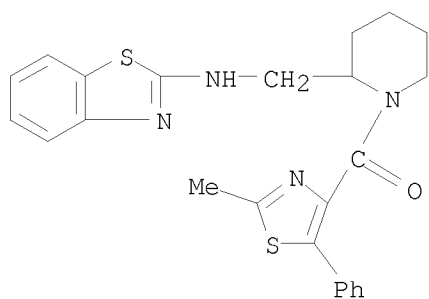
RN 475102-69-3 CAPLUS

CN Methanone, [2-[(2-benzothiazolylamino)methyl]-1-piperidinyl][1,1'-biphenyl]-2-yl- (CA INDEX NAME)



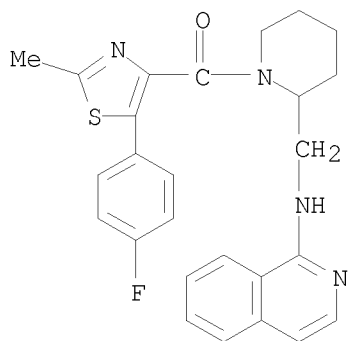
RN 475102-70-6 CAPLUS

CN Methanone, [2-[(2-benzothiazolylamino)methyl]-1-piperidinyl](2-methyl-5-phenyl-4-thiazolyl)- (CA INDEX NAME)



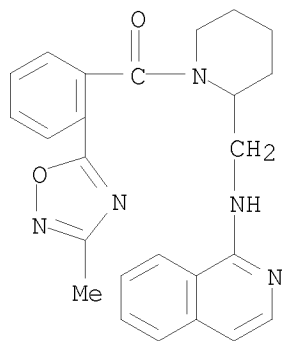
RN 475102-71-7 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][2-[(1-isoquinolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)



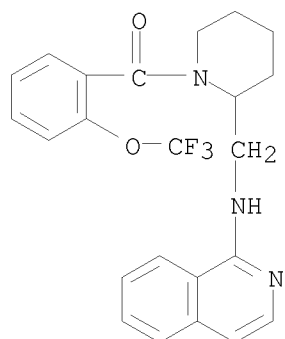
RN 475102-72-8 CAPLUS

CN Methanone, [2-[(1-isoquinolinylamino)methyl]-1-piperidinyl][2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]- (CA INDEX NAME)

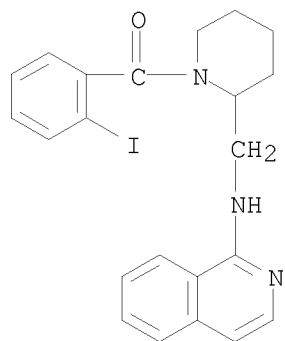


RN 475102-73-9 CAPLUS

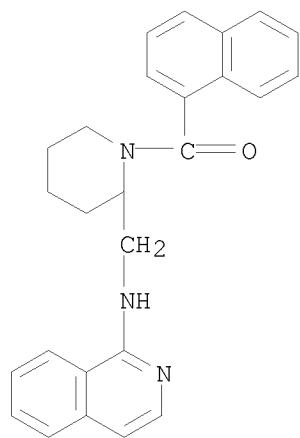
CN Methanone, [2-[(1-isoquinolinylamino)methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



RN 475102-74-0 CAPLUS
 CN Methanone, (2-iodophenyl) [2-[(1-isoquinolinylamino)methyl]-1-piperidinyl]-
 (CA INDEX NAME)

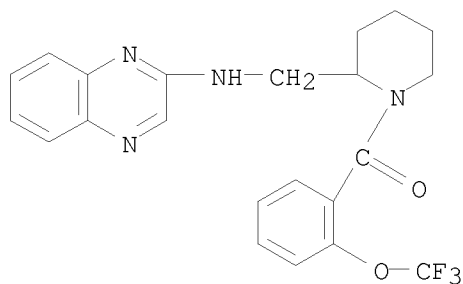


RN 475102-75-1 CAPLUS
 CN Methanone, [2-[(1-isoquinolinylamino)methyl]-1-piperidinyl]-1-naphthalenyl-
 (CA INDEX NAME)



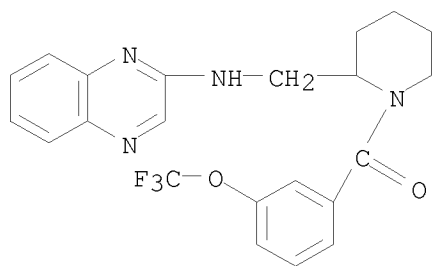
RN 475102-76-2 CAPLUS

CN Methanone, [2-[(2-quinoxalinylamino)methyl]-1-piperidinyll][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



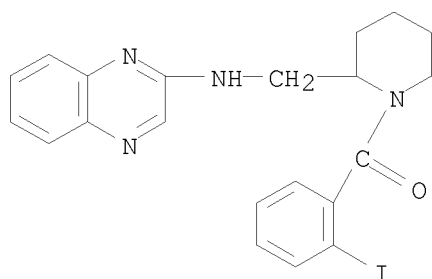
RN 475102-77-3 CAPLUS

CN Methanone, [2-[(2-quinoxalinylamino)methyl]-1-piperidinyll][3-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



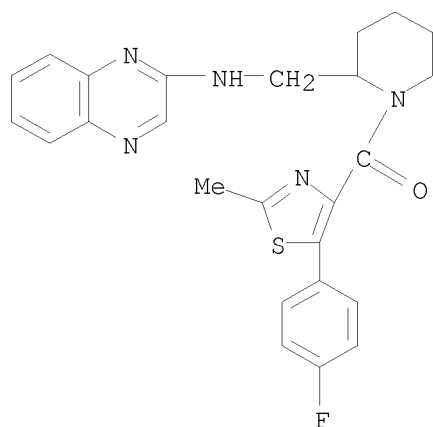
RN 475102-78-4 CAPLUS

CN Methanone, (2-iodophenyl)[2-[(2-quinoxalinylamino)methyl]-1-piperidinyll]- (CA INDEX NAME)



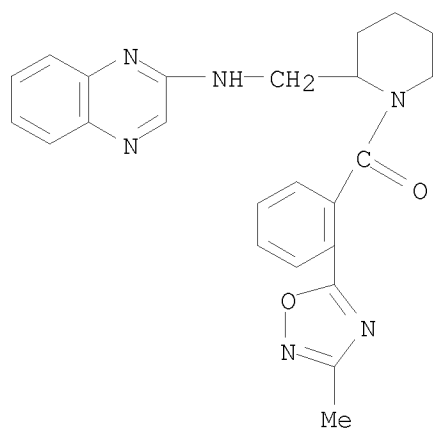
RN 475102-79-5 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][2-[(2-quinoxalinylamino)methyl]-1-piperidinyll]- (CA INDEX NAME)



RN 475102-80-8 CAPLUS

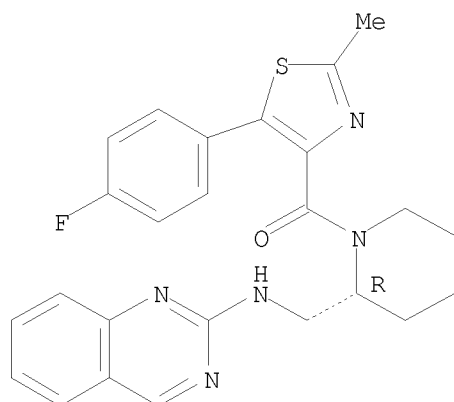
CN Methanone, [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl][2-[(2-quinoxalinylamino)methyl]-1-piperidiny]- (CA INDEX NAME)



RN 475102-82-0 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2R)-2-[(2-quinazolinylamino)methyl]-1-piperidiny]- (CA INDEX NAME)

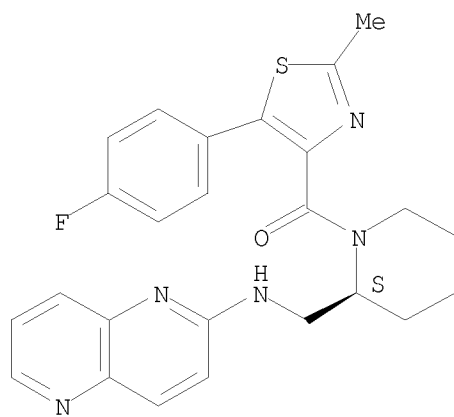
Absolute stereochemistry.



RN 475102-84-2 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[(1,5-naphthyridin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

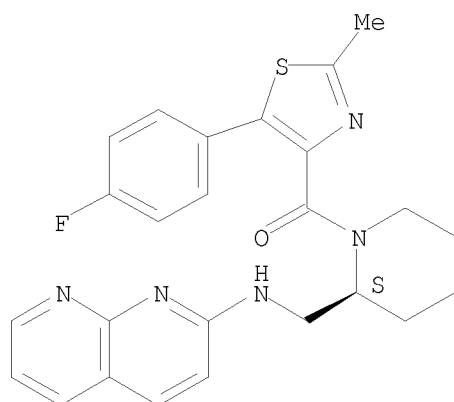
Absolute stereochemistry.



RN 475102-86-4 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[(1,8-naphthyridin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

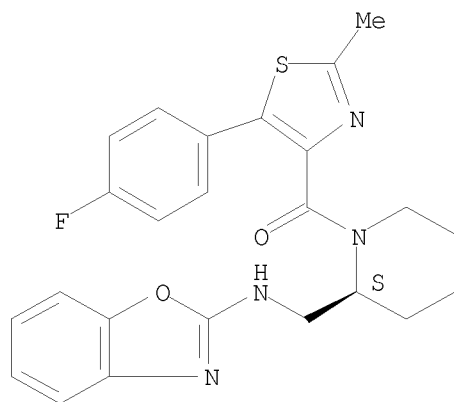
Absolute stereochemistry.



RN 475102-88-6 CAPLUS

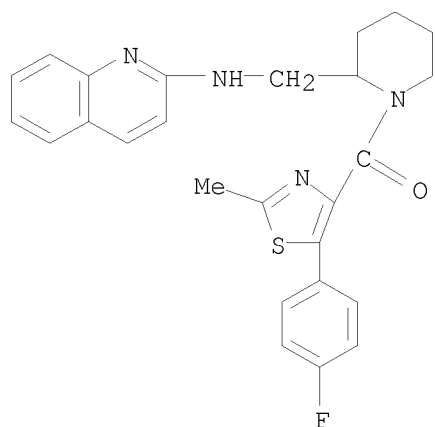
CN Methanone, [(2S)-2-[(2-benzoxazolylamino)methyl]-1-piperidinyl][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.

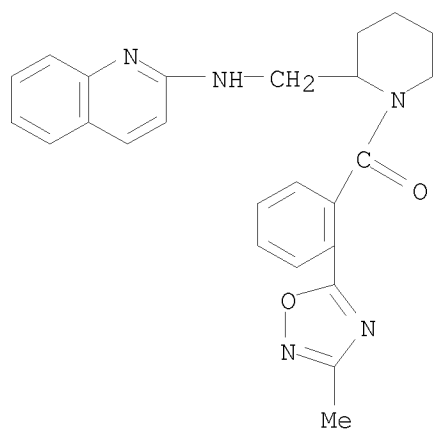


RN 475102-90-0 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][2-[(2-quinolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

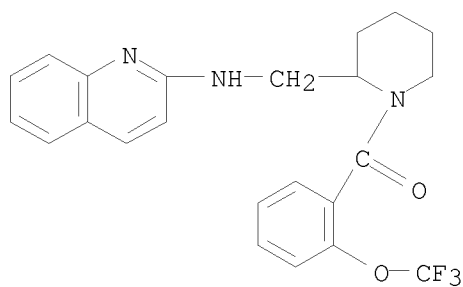


RN 475102-91-1 CAPLUS
 CN Methanone, [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl][2-[(2-quinolinylamino)methyl]-1-piperidinyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

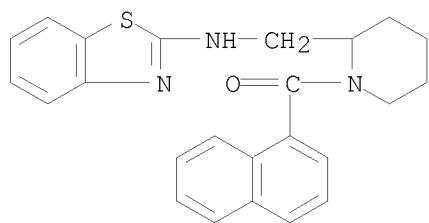
RN 475102-92-2 CAPLUS
 CN Methanone, [2-[(2-quinolinylamino)methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 475102-93-3 CAPLUS

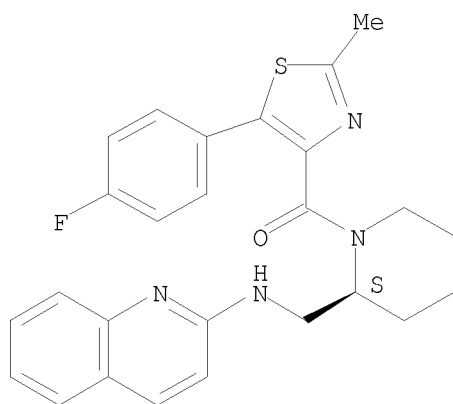
CN Methanone, [2-[(2-benzothiazolylamino)methyl]-1-piperidinyl]-1-naphthalenyl- (CA INDEX NAME)



RN 475102-94-4 CAPLUS

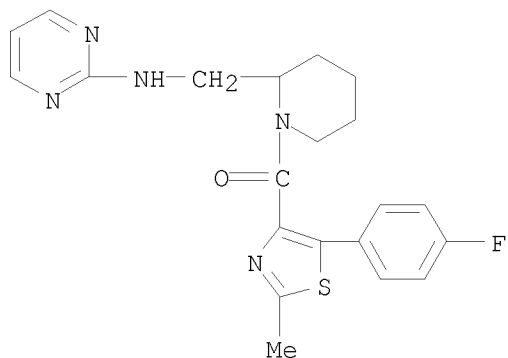
CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[(2-quinolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



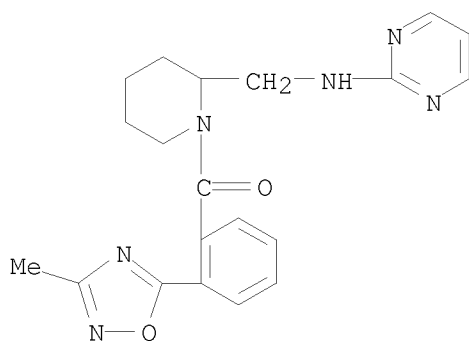
RN 475102-95-5 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][2-[(2-pyrimidinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)



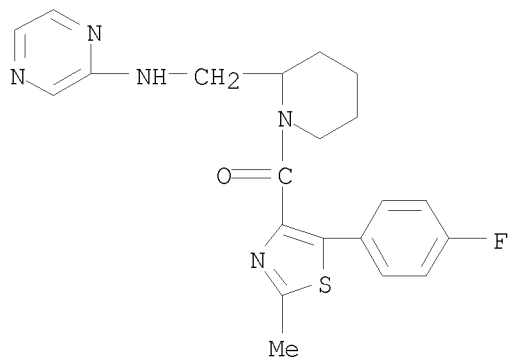
RN 475102-96-6 CAPLUS

CN Methanone, [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl][2-[(2-pyrimidinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)



RN 475102-97-7 CAPLUS

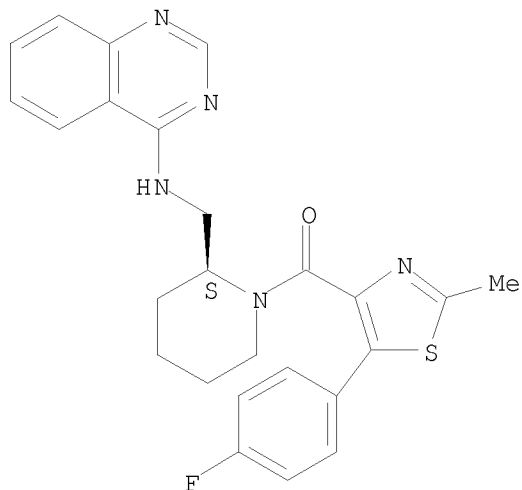
CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][2-[(2-pyrazinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)



RN 475102-98-8 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

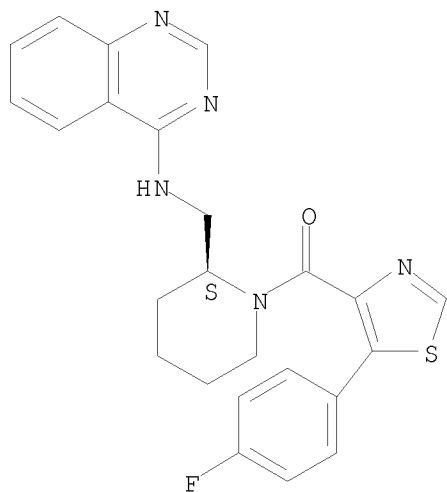
Absolute stereochemistry.



RN 475103-00-5 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-4-thiazolyl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

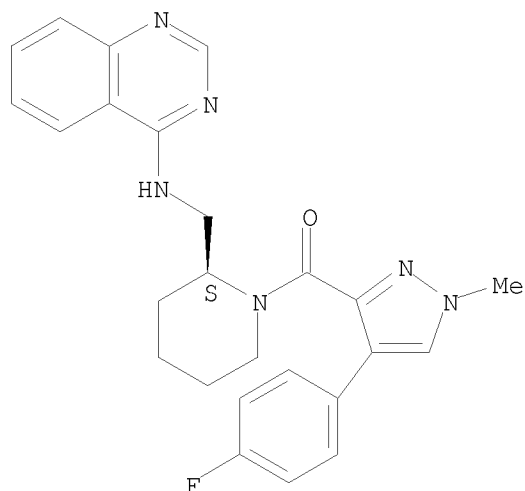
Absolute stereochemistry.



RN 475103-02-7 CAPLUS

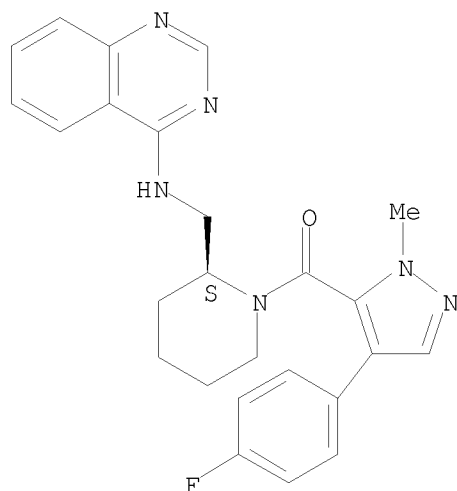
CN Methanone, [4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



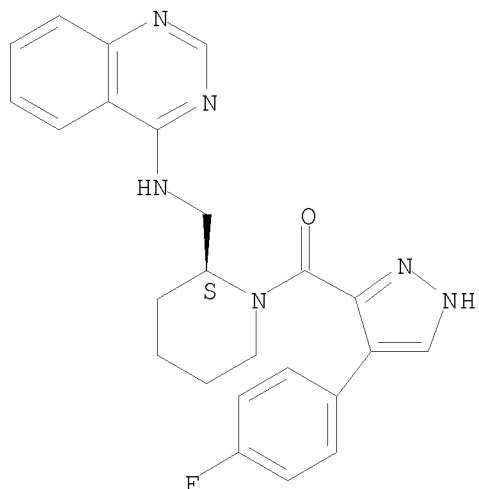
RN 475103-03-8 CAPLUS
 CN Methanone, [4-(4-fluorophenyl)-1-methyl-1H-pyrazol-5-yl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



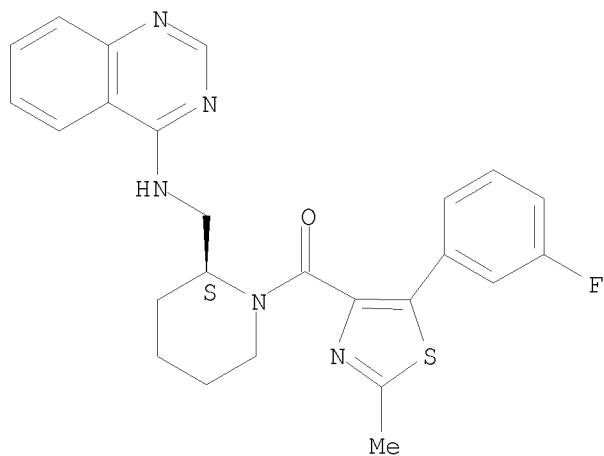
RN 475103-05-0 CAPLUS
 CN Methanone, [4-(4-fluorophenyl)-1H-pyrazol-3-yl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



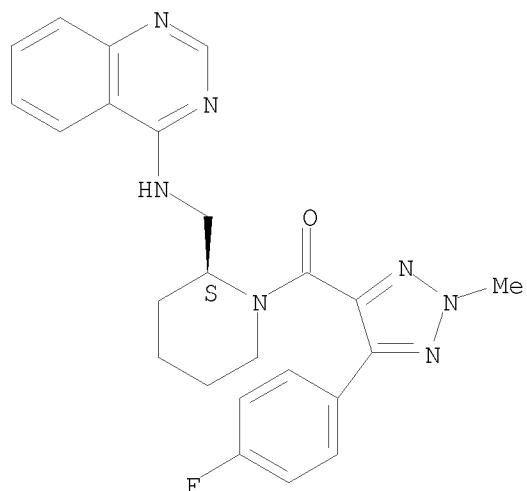
RN 475103-06-1 CAPLUS
 CN Methanone, [5-(3-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidiny]- (CA INDEX NAME)

Absolute stereochemistry.



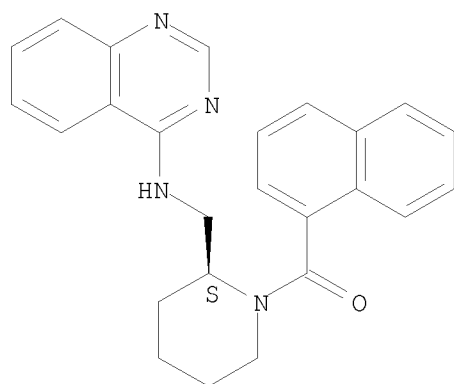
RN 475103-07-2 CAPLUS
 CN Methanone, [5-(4-fluorophenyl)-2-methyl-2H-1,2,3-triazol-4-yl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidiny]- (CA INDEX NAME)

Absolute stereochemistry.



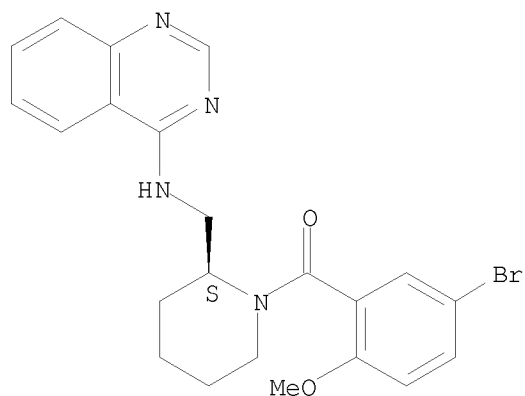
RN 475103-08-3 CAPLUS
 CN Methanone, 1-naphthalenyl[(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-09-4 CAPLUS
 CN Methanone, (5-bromo-2-methoxyphenyl)[(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

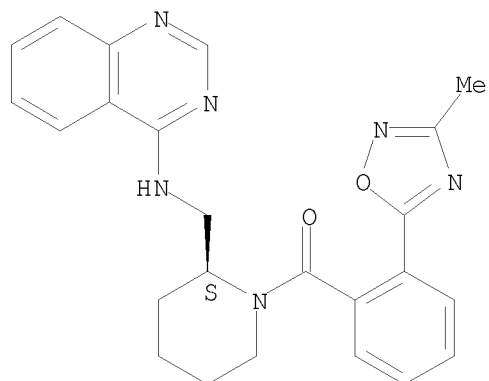
Absolute stereochemistry.



RN 475103-10-7 CAPLUS

CN Methanone, [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl][(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

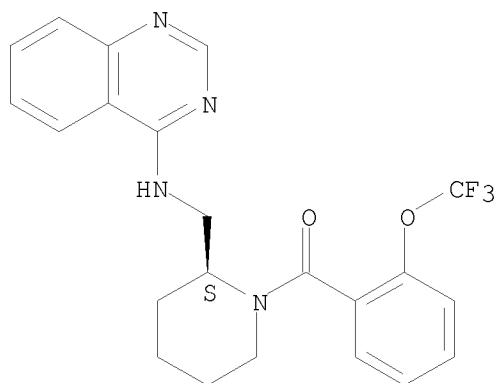
Absolute stereochemistry.



RN 475103-11-8 CAPLUS

CN Methanone, [(2S)-2-[(4-quinazolinylamino)methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

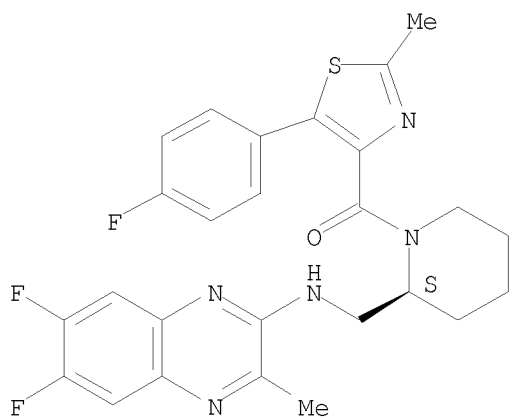
Absolute stereochemistry.



RN 475103-12-9 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-3-methyl-2-quinoxaliny]amino]methyl]-1-piperidiny][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)

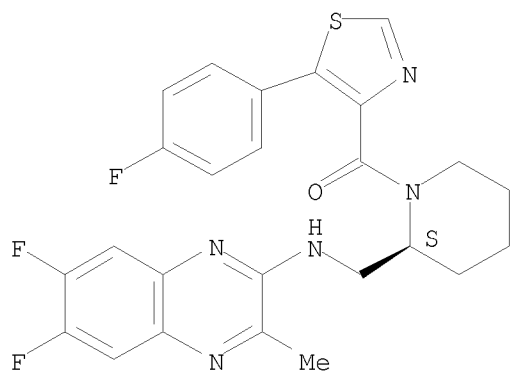
Absolute stereochemistry.



RN 475103-13-0 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-3-methyl-2-quinoxaliny]amino]methyl]-1-piperidiny][5-(4-fluorophenyl)-4-thiazolyl]- (CA INDEX NAME)

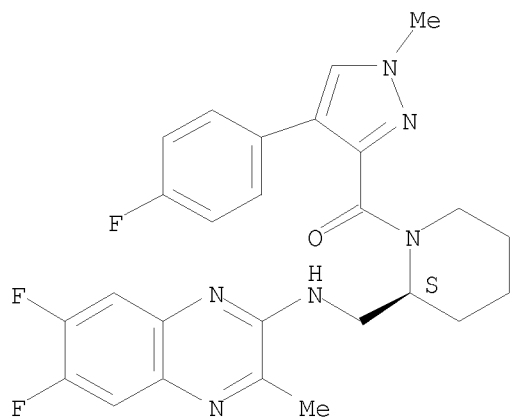
Absolute stereochemistry.



RN 475103-14-1 CAPLUS

CN Methanone, [(2S)-2-[[[(6,7-difluoro-3-methyl-2-quinoxalinyloxy)methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (CA INDEX NAME)

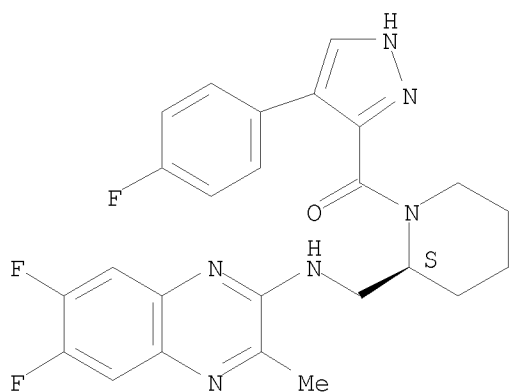
Absolute stereochemistry.



RN 475103-15-2 CAPLUS

CN Methanone, [(2S)-2-[[[(6,7-difluoro-3-methyl-2-quinoxalinyloxy)methyl]-1-piperidinyl][4-(4-fluorophenyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

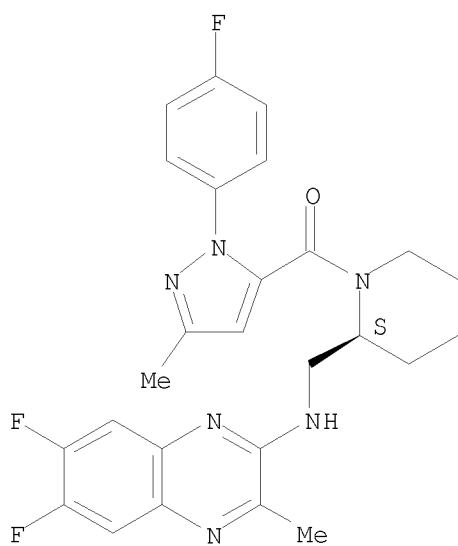
Absolute stereochemistry.



RN 475103-16-3 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-3-methyl-2-quinoxaliny]amino]methyl]-1-piperidinyl][1-(4-fluorophenyl)-3-methyl-1H-pyrazol-5-yl]- (CA INDEX NAME)

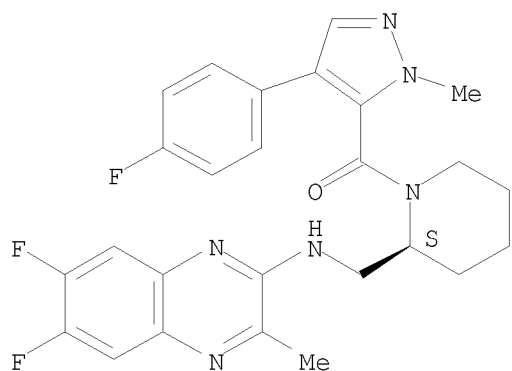
Absolute stereochemistry.



RN 475103-17-4 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-3-methyl-2-quinoxaliny]amino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-5-yl]- (CA INDEX NAME)

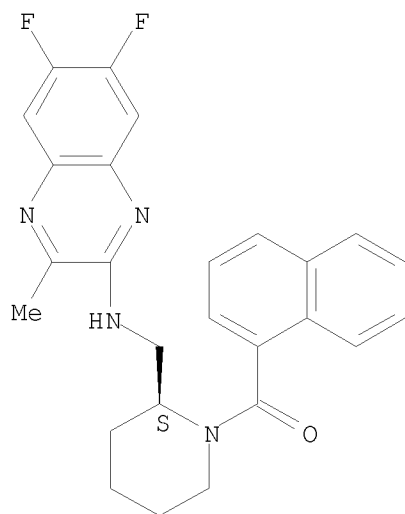
Absolute stereochemistry.



RN 475103-18-5 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-3-methyl-2-quinoxaliny]amino]methyl]-1-piperidinyl]-1-naphthalenyl- (CA INDEX NAME)

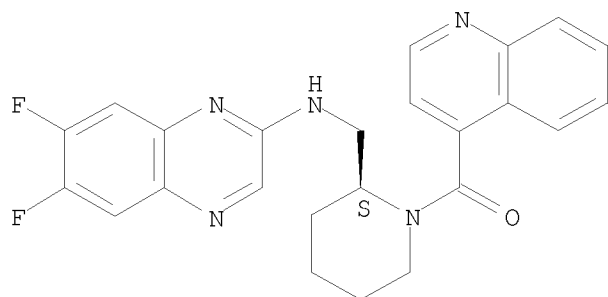
Absolute stereochemistry.



RN 475103-19-6 CAPLUS

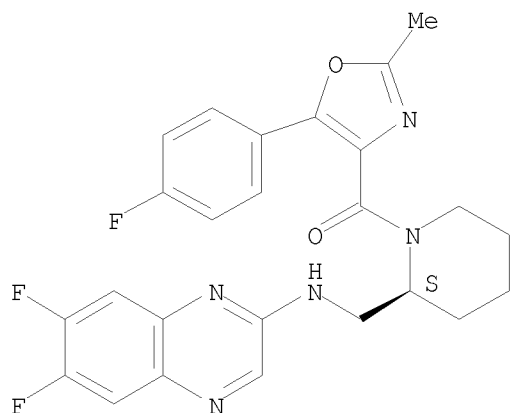
CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl]-4-quinolinyl- (CA INDEX NAME)

Absolute stereochemistry.



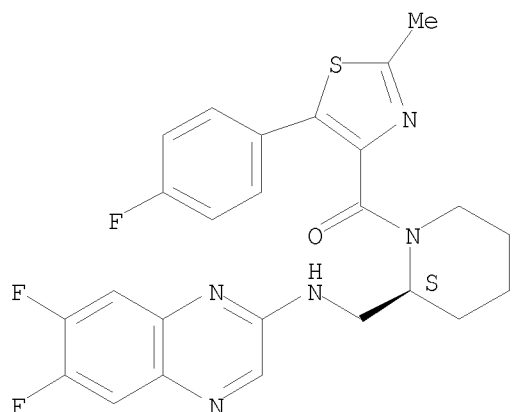
RN 475103-20-9 CAPLUS
 CN Methanone, [(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)methyl]-1-piperidinyloxy][5-(4-fluorophenyl)-2-methyl-4-oxazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-21-0 CAPLUS
 CN Methanone, [(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)methyl]-1-piperidinyloxy][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)

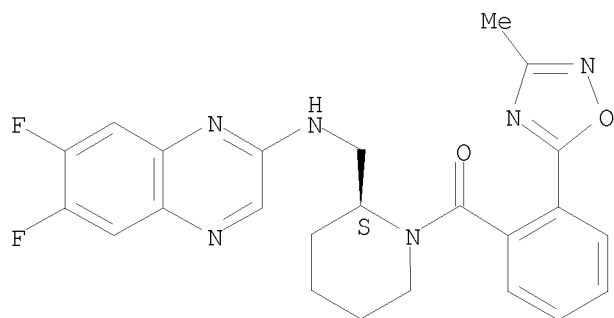
Absolute stereochemistry.



RN 475103-22-1 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl][2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]- (CA INDEX NAME)

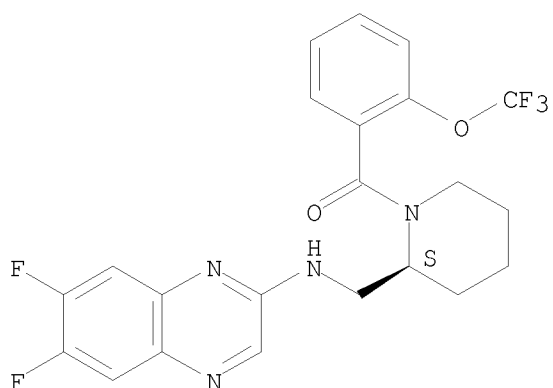
Absolute stereochemistry.



RN 475103-23-2 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

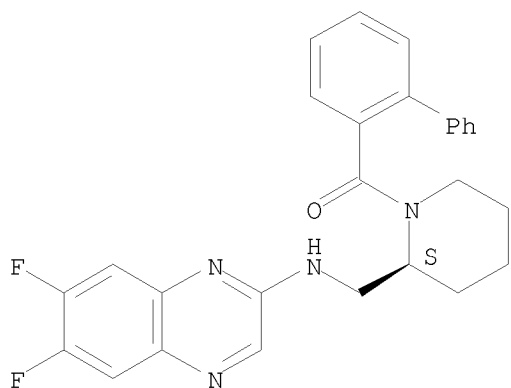
Absolute stereochemistry.



RN 475103-24-3 CAPLUS

CN Methanone, [1,1'-biphenyl]-2-yl[(2S)-2-[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyl]- (CA INDEX NAME)

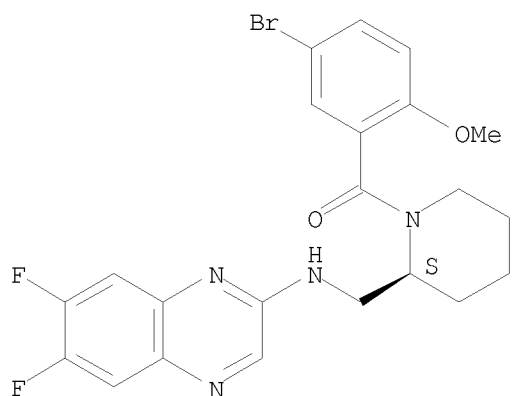
Absolute stereochemistry.



RN 475103-25-4 CAPLUS

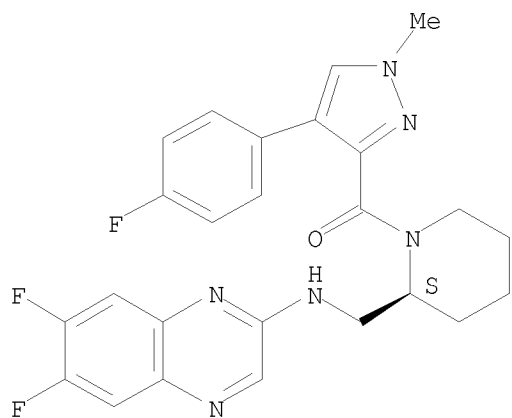
CN Methanone, (5-bromo-2-methoxyphenyl)[(2S)-2-[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



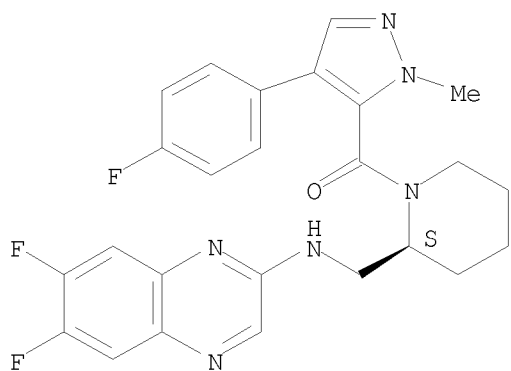
RN 475103-26-5 CAPLUS
 CN Methanone, [(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)amino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-27-6 CAPLUS
 CN Methanone, [(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)amino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-5-yl]- (CA INDEX NAME)

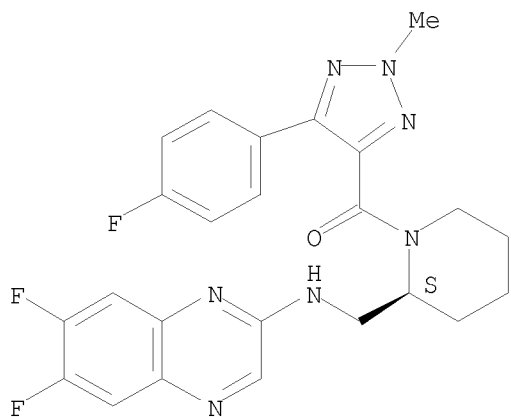
Absolute stereochemistry.



RN 475103-29-8 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyl][5-(4-fluorophenyl)-2-methyl-2H-1,2,3-triazol-4-yl]- (CA INDEX NAME)

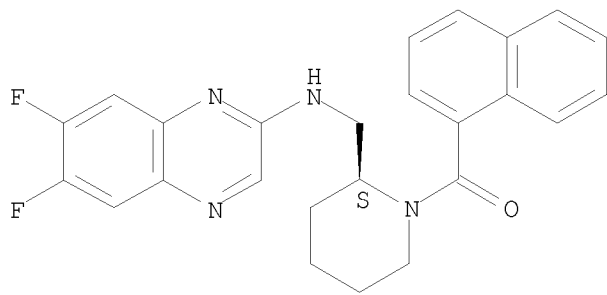
Absolute stereochemistry.



RN 475103-30-1 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyl]-1-naphthalenyl- (CA INDEX NAME)

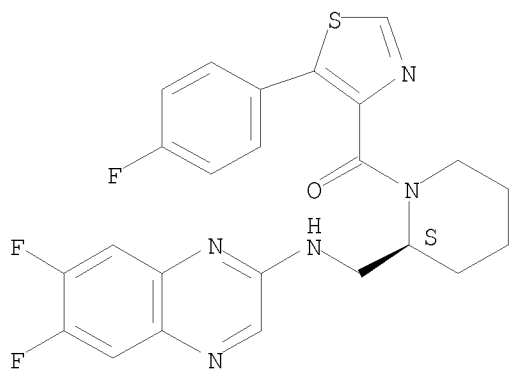
Absolute stereochemistry.



RN 475103-31-2 CAPLUS

CN Methanone, [(2S)-2-[[(6,7-difluoro-2-quinoxaliny)amino]methyl]-1-piperidiny] [5-(4-fluorophenyl)-4-thiazolyl]- (CA INDEX NAME)

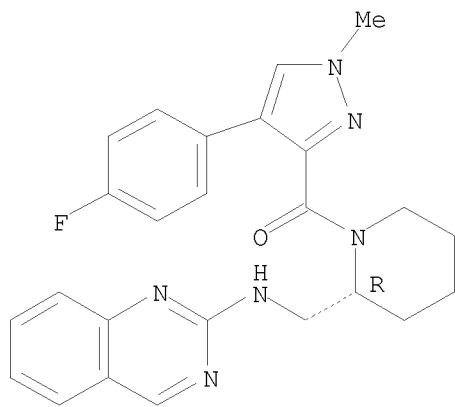
Absolute stereochemistry.



RN 475103-32-3 CAPLUS

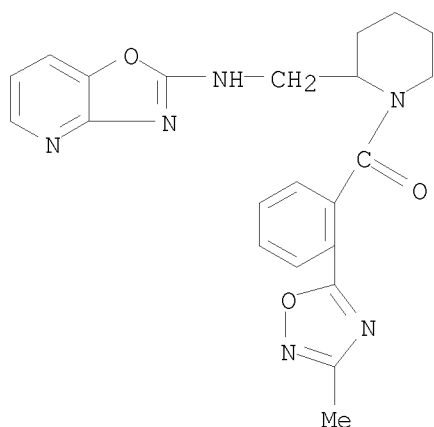
CN Methanone, [4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl] [(2R)-2-[(2-quinazolinylamino)methyl]-1-piperidiny]- (CA INDEX NAME)

Absolute stereochemistry.



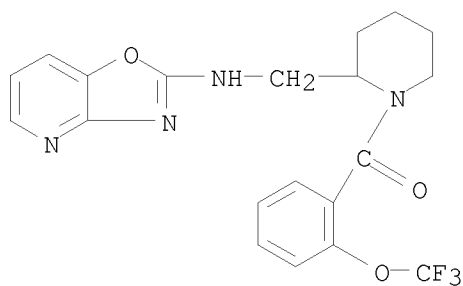
RN 475103-33-4 CAPLUS

CN Methanone, [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl] [2-[(oxazolo[4,5-b]pyridin-2-ylamino)methyl]-1-piperidiny]- (CA INDEX NAME)



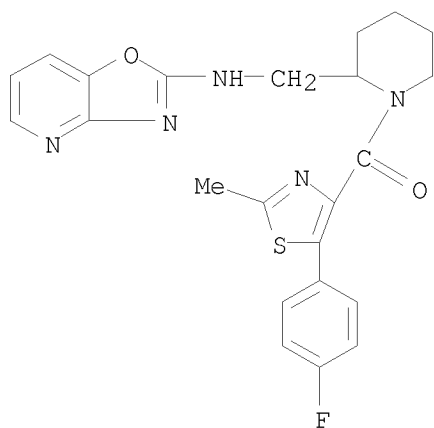
RN 475103-34-5 CAPLUS

CN Methanone, [2-[(oxazolo[4,5-b]pyridin-2-ylamino)methyl]-1-piperidinyl][2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



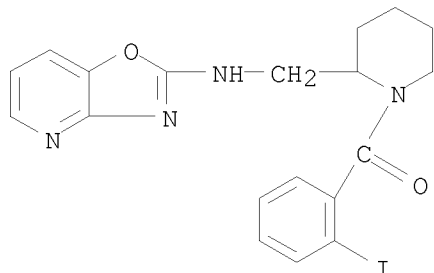
RN 475103-35-6 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][2-[(oxazolo[4,5-b]pyridin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)



RN 475103-36-7 CAPLUS

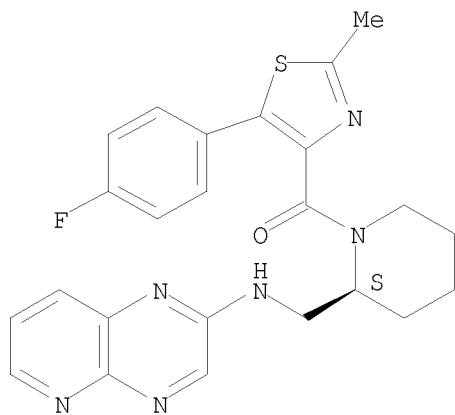
CN Methanone, (2-iodophenyl)[2-[(oxazolo[4,5-b]pyridin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)



RN 475103-40-3 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[(pyrido[2,3-b]pyrazin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

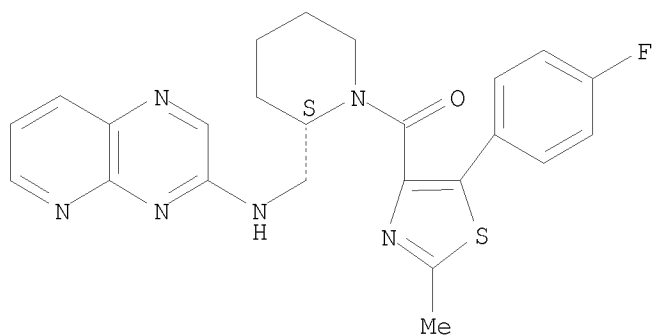
Absolute stereochemistry.



RN 475103-41-4 CAPLUS

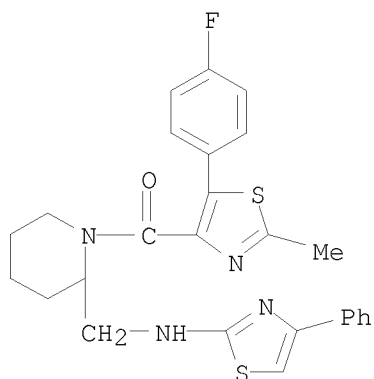
CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[(pyrido[2,3-b]pyrazin-3-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-42-5 CAPLUS

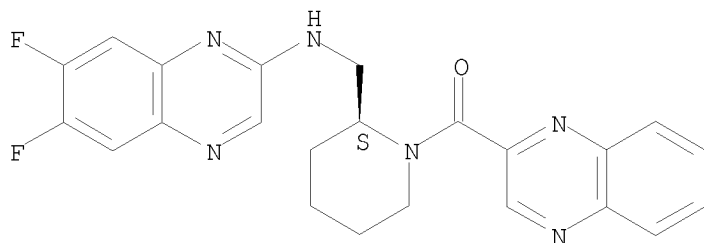
CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][2-[(4-phenyl-2-thiazolyl)amino]methyl]-1-piperidinyl- (CA INDEX NAME)



RN 475103-43-6 CAPLUS

CN Methanone, [(2S)-2-[(6,7-difluoro-2-quinoxaliny)amino]methyl]-1-piperidinyl]-2-quinoxaliny- (CA INDEX NAME)

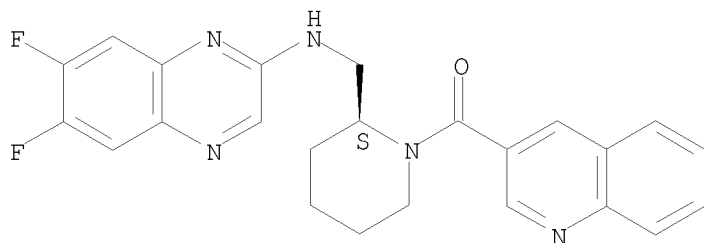
Absolute stereochemistry.



RN 475103-44-7 CAPLUS

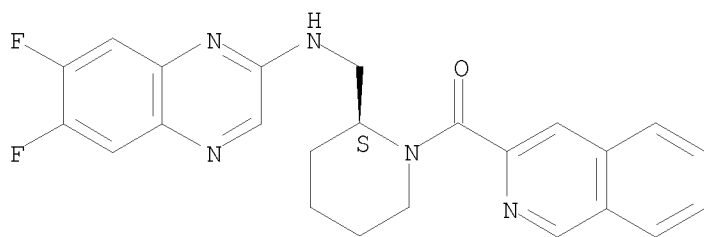
CN Methanone, [(2S)-2-[(6,7-difluoro-2-quinoxaliny)amino]methyl]-1-piperidinyl]-3-quinoliny- (CA INDEX NAME)

Absolute stereochemistry.



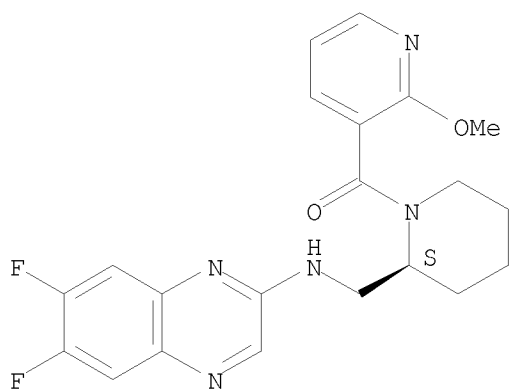
RN 475103-45-8 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl]-3-isoquinoliny- (CA INDEX NAME)

Absolute stereochemistry.



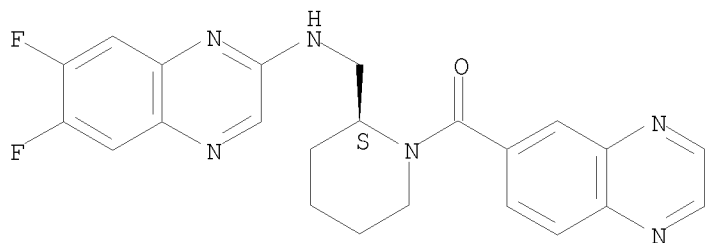
RN 475103-46-9 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl](2-methoxy-3-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-47-0 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl]-6-quinoxaliny- (CA INDEX NAME)

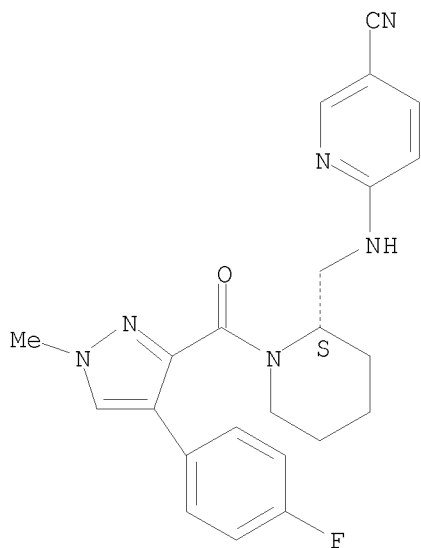
Absolute stereochemistry.



RN 475103-48-1 CAPLUS

CN 3-Pyridinecarbonitrile, 6-[[[(2S)-1-[[4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

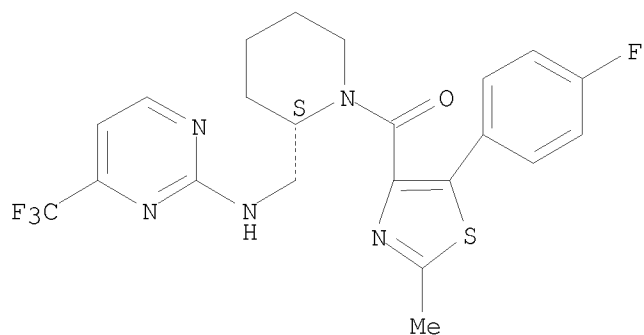
Absolute stereochemistry.



RN 475103-49-2 CAPLUS

CN Methanone, [5-(4-fluorophenyl)-2-methyl-4-thiazolyl][(2S)-2-[[[4-(trifluoromethyl)-2-pyrimidinyl]amino]methyl]-1-piperidinyl]- (CA INDEX NAME)

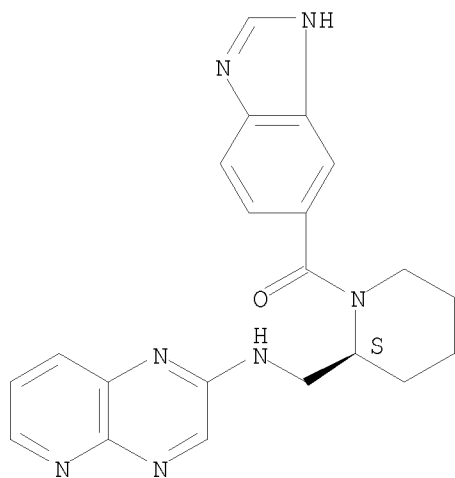
Absolute stereochemistry.



RN 475103-50-5 CAPLUS

CN Methanone, 1H-benzimidazol-6-yl[(2S)-2-[(pyrido[2,3-b]pyrazin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

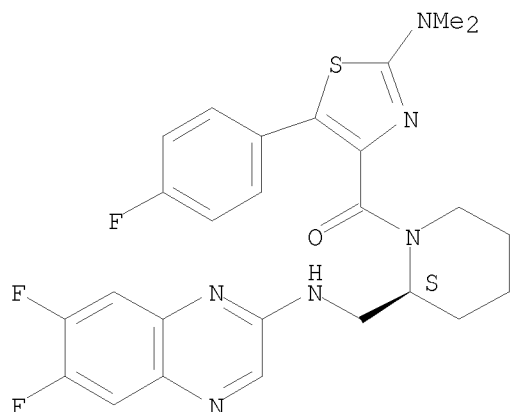
Absolute stereochemistry.



RN 475103-51-6 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl][2-(dimethylamino)-5-(4-fluorophenyl)-4-thiazolyl]- (CA INDEX NAME)

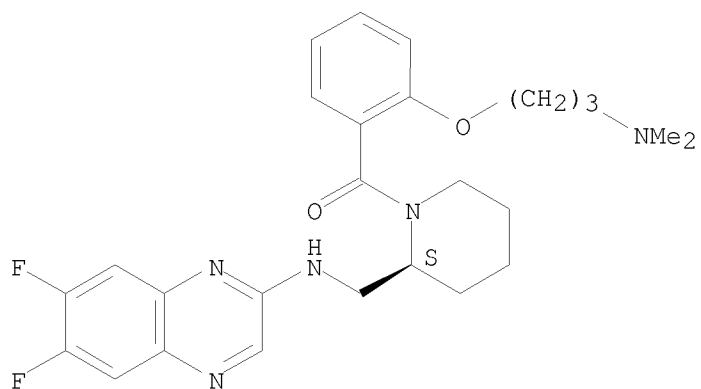
Absolute stereochemistry.



RN 475103-52-7 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidiny][2-[3-(dimethylamino)propoxy]phenyl]- (CA INDEX NAME)

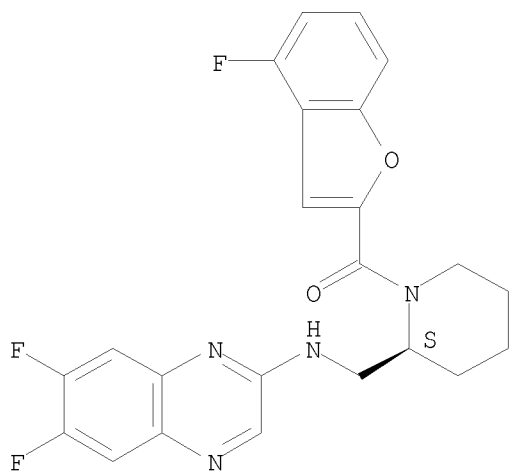
Absolute stereochemistry.



RN 475103-53-8 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidiny](4-fluoro-2-benzofuranyl)- (CA INDEX NAME)

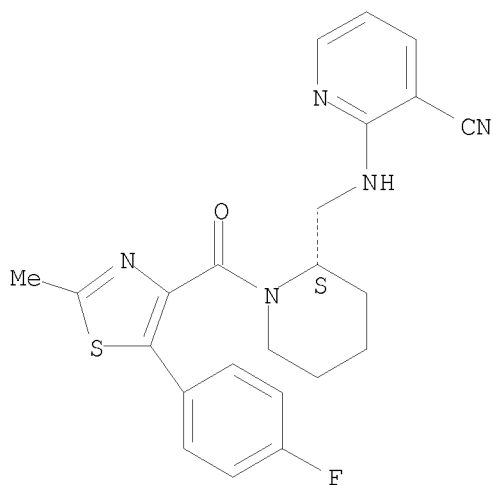
Absolute stereochemistry.



RN 475103-54-9 CAPLUS

CN 3-Pyridinecarbonitrile, 2-[[[(2S)-1-[[5-(4-fluorophenyl)-2-methyl-4-thiazolyl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

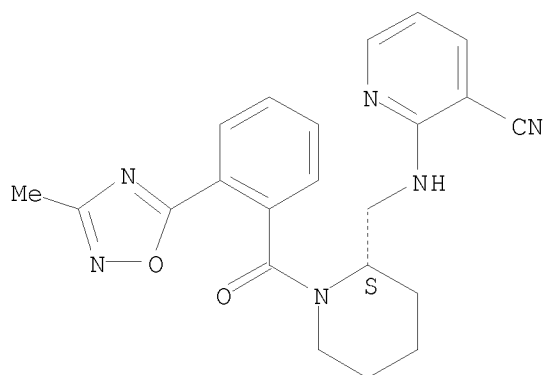
Absolute stereochemistry.



RN 475103-55-0 CAPLUS

CN 3-Pyridinecarbonitrile, 2-[[[(2S)-1-[2-(3-methyl-1,2,4-oxadiazol-5-yl)benzoyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

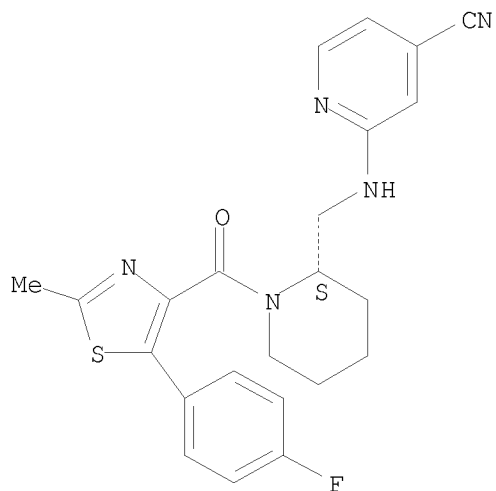
Absolute stereochemistry.



RN 475103-56-1 CAPLUS

CN 4-Pyridinecarbonitrile, 2-[[[(2S)-1-[[5-(4-fluorophenyl)-2-methyl-4-thiazolyl]carbonyl]-2-piperidiny]methyl]amino]- (CA INDEX NAME)

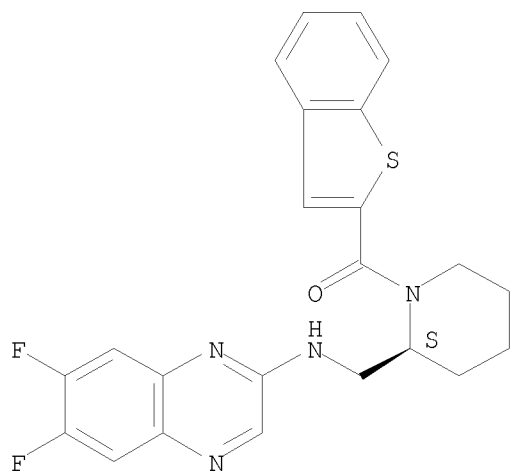
Absolute stereochemistry.



RN 475103-57-2 CAPLUS

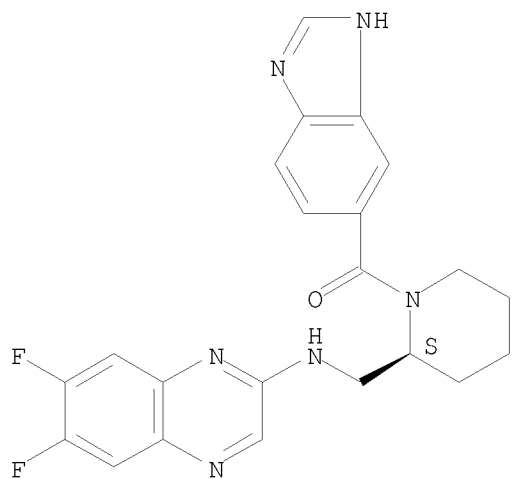
CN Methanone, benzo[b]thien-2-yl[(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidiny]- (CA INDEX NAME)

Absolute stereochemistry.



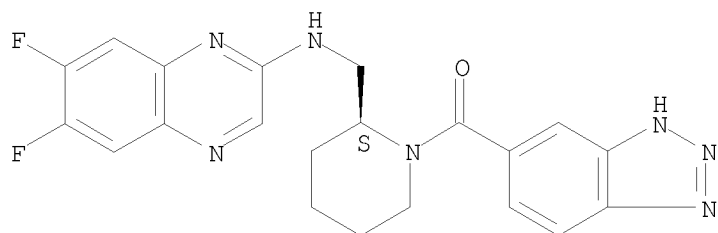
RN 475103-58-3 CAPLUS
 CN Methanone, 1H-benzimidazol-6-yl[(2S)-2-[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyloxy- (CA INDEX NAME)

Absolute stereochemistry.



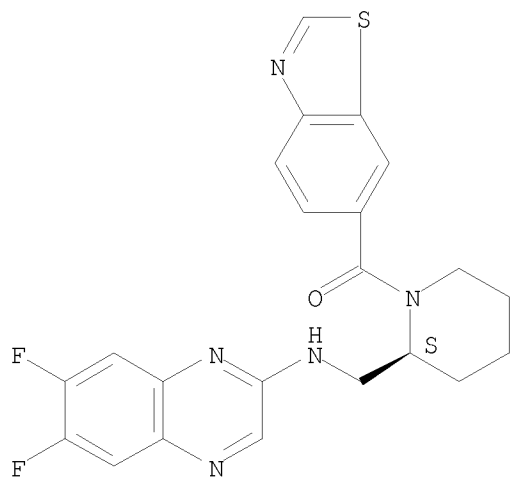
RN 475103-59-4 CAPLUS
 CN Methanone, 1H-benzotriazol-6-yl[(2S)-2-[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyloxy- (CA INDEX NAME)

Absolute stereochemistry.



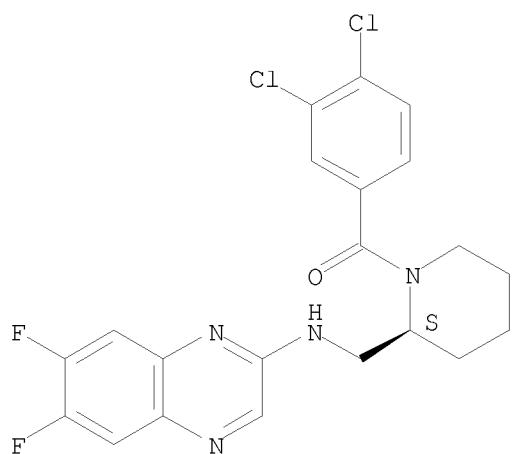
RN 475103-60-7 CAPLUS
 CN Methanone, 6-benzothiazolyl[(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)methyl]-(1-piperidinyl)]- (CA INDEX NAME)

Absolute stereochemistry.



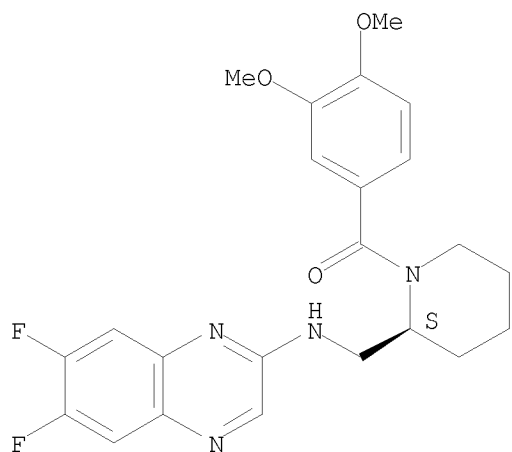
RN 475103-61-8 CAPLUS
 CN Methanone, (3,4-dichlorophenyl)[(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)methyl]-(1-piperidinyl)]- (CA INDEX NAME)

Absolute stereochemistry.



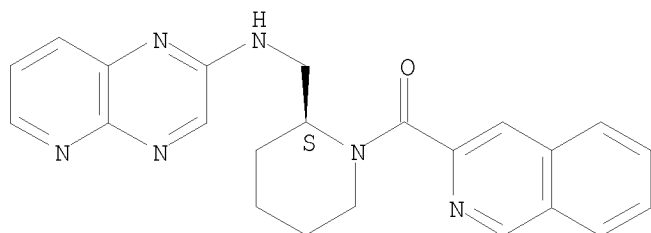
RN 475103-62-9 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl](3,4-dimethoxyphenyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-63-0 CAPLUS
 CN Methanone, 3-isoquinolinyl[(2S)-2-[(pyrido[2,3-b]pyrazin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

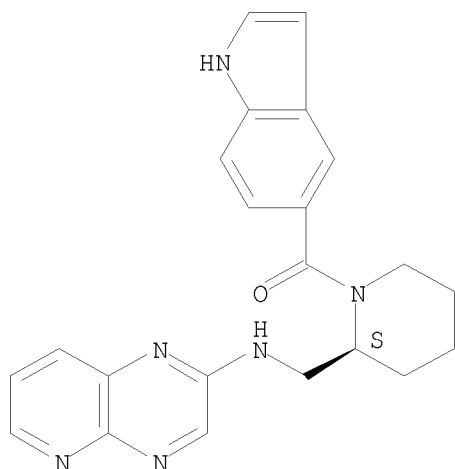
Absolute stereochemistry.



RN 475103-64-1 CAPLUS

CN Methanone, 1H-indol-5-yl[(2S)-2-[(pyrido[2,3-b]pyrazin-2-ylamino)methyl]-1-piperidiny]- (CA INDEX NAME)

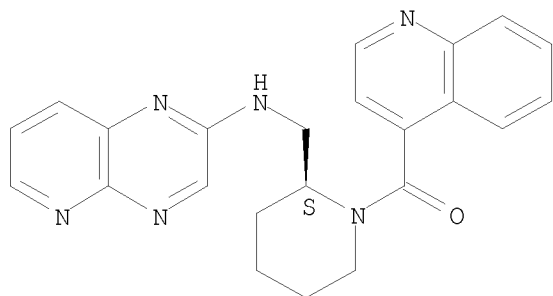
Absolute stereochemistry.



RN 475103-65-2 CAPLUS

CN Methanone, [(2S)-2-[(pyrido[2,3-b]pyrazin-2-ylamino)methyl]-1-piperidiny]-4-quinolinyl- (CA INDEX NAME)

Absolute stereochemistry.

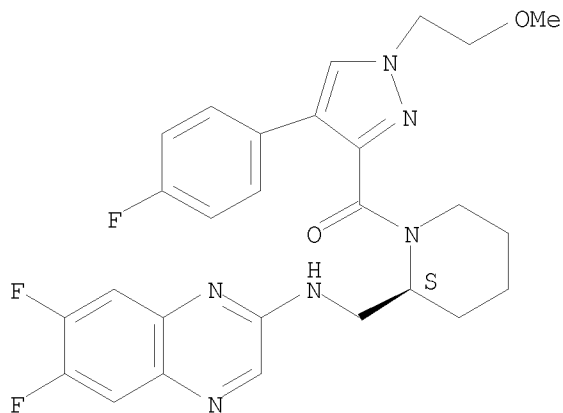


RN 475103-66-3 CAPLUS

CN Methanone, [(2S)-2-[[6,7-difluoro-2-quinoxaliny)amino]methyl]-1-

piperidinyll[4-(4-fluorophenyl)-1-(2-methoxyethyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

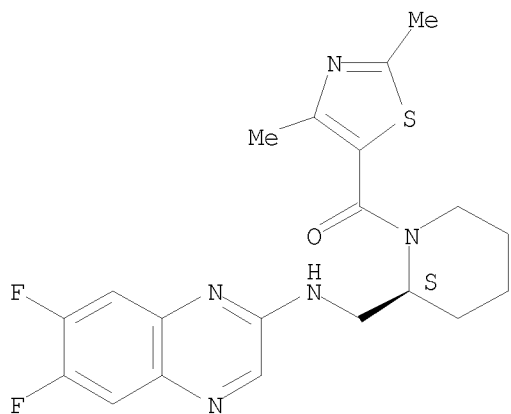
Absolute stereochemistry.



RN 475103-67-4 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyll(2,4-dimethyl-5-thiazolyl)- (CA INDEX NAME)

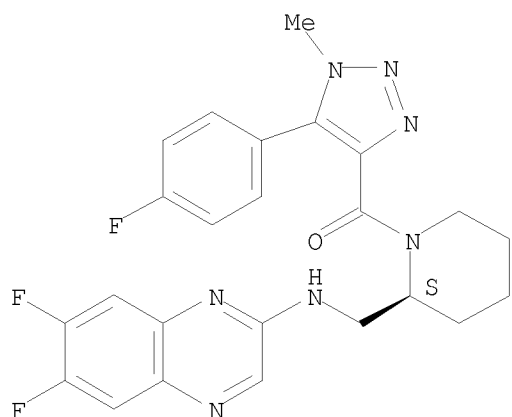
Absolute stereochemistry.



RN 475103-68-5 CAPLUS

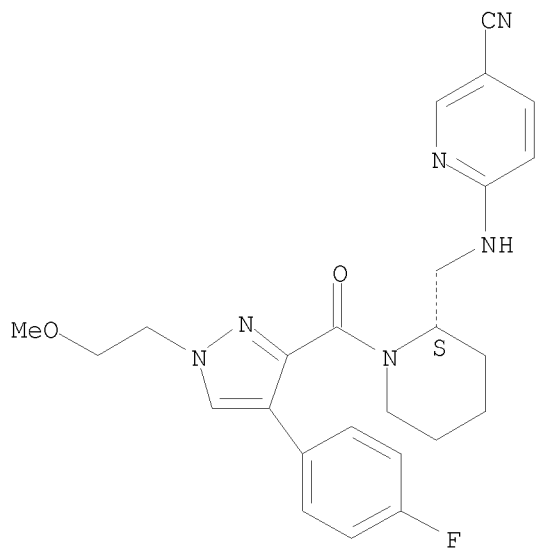
CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyll[5-(4-fluorophenyl)-1-methyl-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)

Absolute stereochemistry.



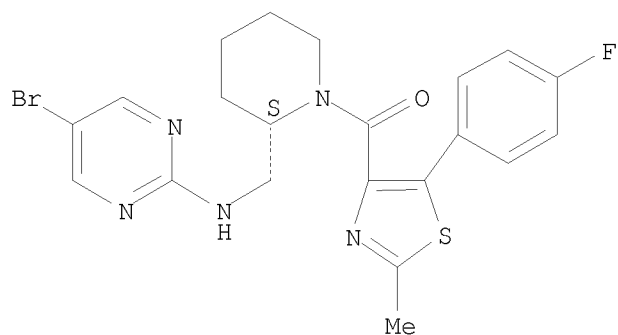
RN 475103-69-6 CAPLUS
 CN 3-Pyridinecarbonitrile, 6-[[[(2S)-1-[[4-(4-fluorophenyl)-1-(2-methoxyethyl)-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-70-9 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)

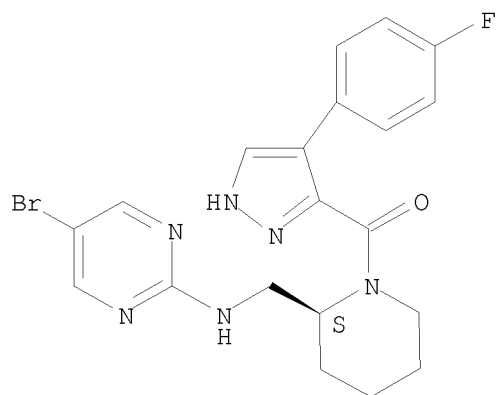
Absolute stereochemistry.



RN 475103-71-0 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

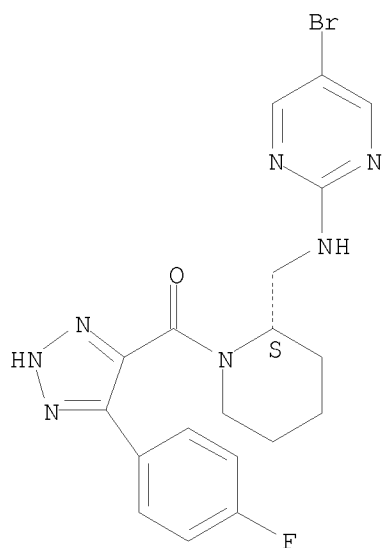
Absolute stereochemistry.



RN 475103-72-1 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][5-(4-fluorophenyl)-2H-1,2,3-triazol-4-yl]- (CA INDEX NAME)

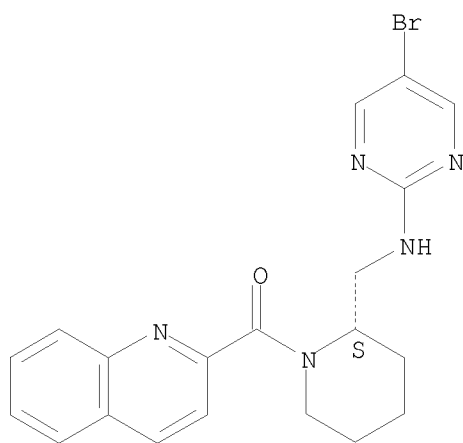
Absolute stereochemistry.



RN 475103-73-2 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl]-2-quinolinyl]- (CA INDEX NAME)

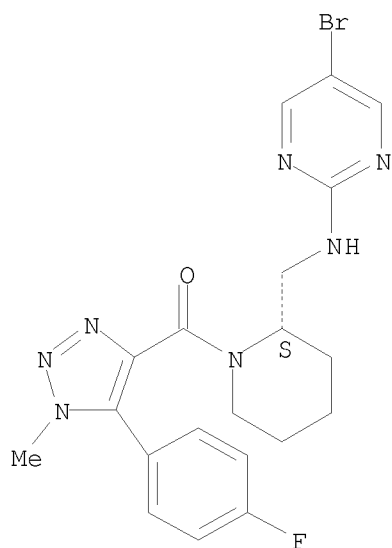
Absolute stereochemistry.



RN 475103-74-3 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][5-(4-fluorophenyl)-1-methyl-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)

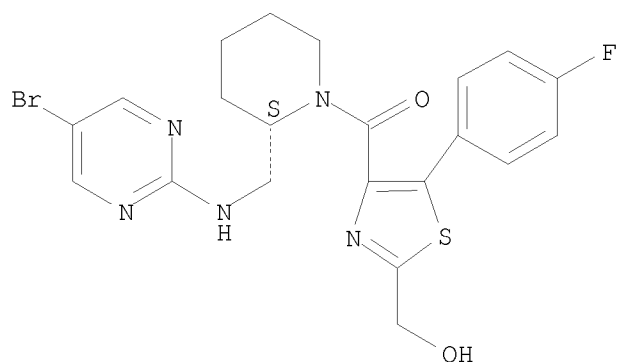
Absolute stereochemistry.



RN 475103-75-4 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][5-(4-fluorophenyl)-2-(hydroxymethyl)-4-thiazolyl]- (CA INDEX NAME)

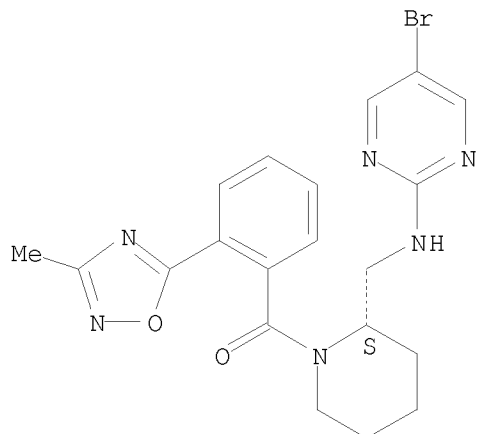
Absolute stereochemistry.



RN 475103-76-5 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]- (CA INDEX NAME)

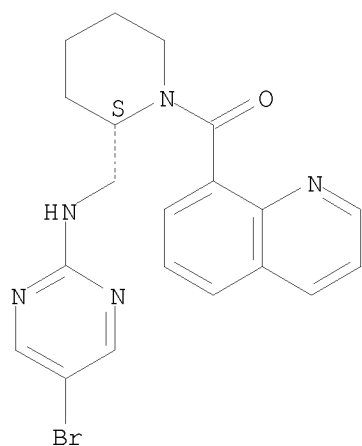
Absolute stereochemistry.



RN 475103-77-6 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl]-8-quinolinyl]- (CA INDEX NAME)

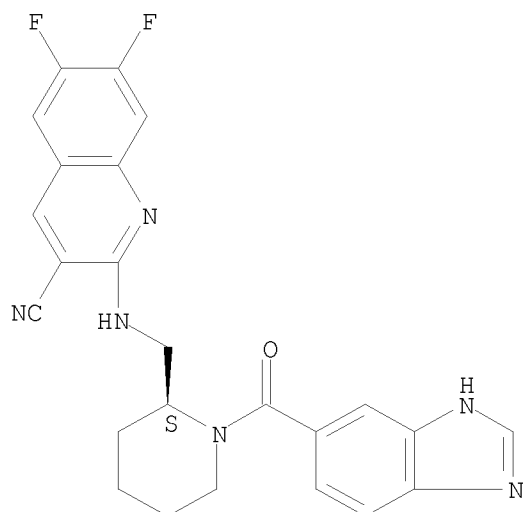
Absolute stereochemistry.



RN 475103-78-7 CAPLUS

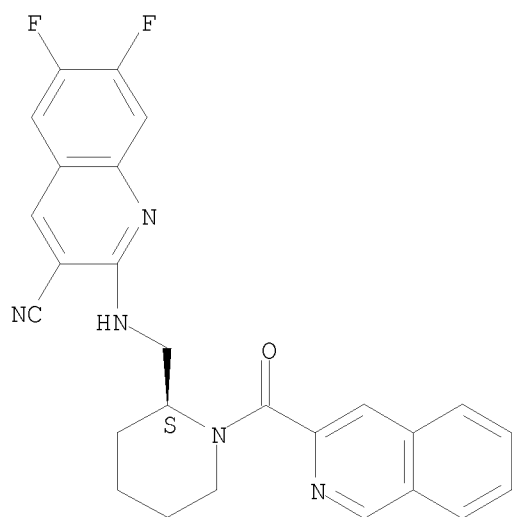
CN 3-Quinolinecarbonitrile, 2-[[[(2S)-1-(1H-benzimidazol-6-ylcarbonyl)-2-piperidinyl]methyl]amino]-6,7-difluoro- (CA INDEX NAME)

Absolute stereochemistry.



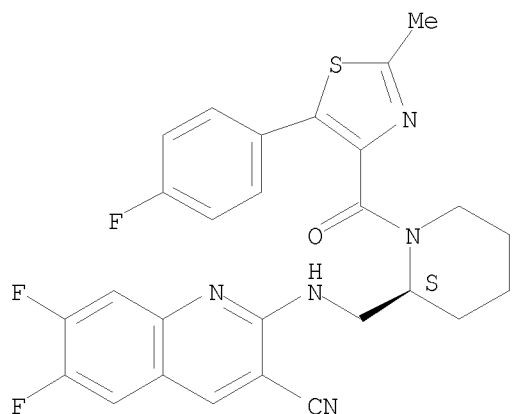
RN 475103-79-8 CAPLUS
 CN 3-Quinolinecarbonitrile, 6,7-difluoro-2-[[[(2S)-1-(3-isoquinolinylcarbonyl)-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-80-1 CAPLUS
 CN 3-Quinolinecarbonitrile, 6,7-difluoro-2-[[[(2S)-1-[[5-(4-fluorophenyl)-2-methyl-4-thiazolyl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

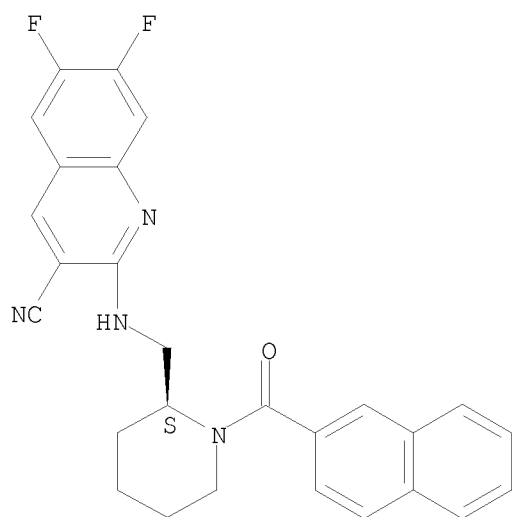
Absolute stereochemistry.



RN 475103-81-2 CAPLUS

CN 3-Quinolinecarbonitrile, 6,7-difluoro-2-[[[(2S)-1-(2-naphthalenylcarbonyl)-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

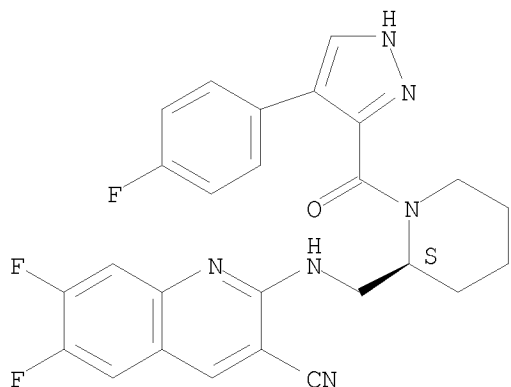
Absolute stereochemistry.



RN 475103-82-3 CAPLUS

CN 3-Quinolinecarbonitrile, 6,7-difluoro-2-[[[(2S)-1-[[4-(4-fluorophenyl)-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

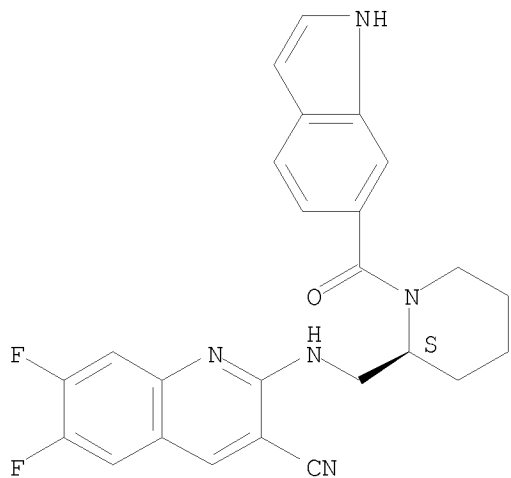
Absolute stereochemistry.



RN 475103-83-4 CAPLUS

CN 3-Quinolinecarbonitrile, 6,7-difluoro-2-[[[(2S)-1-(1H-indol-6-ylcarbonyl)-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

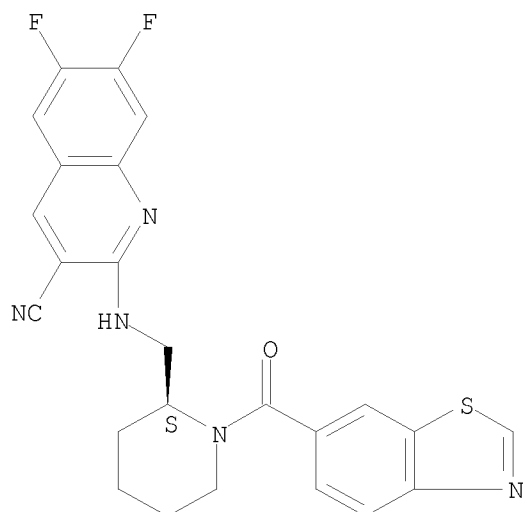
Absolute stereochemistry.



RN 475103-84-5 CAPLUS

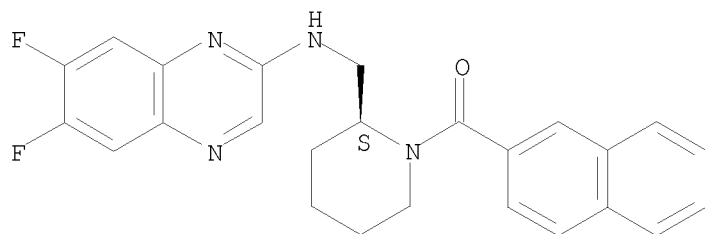
CN 3-Quinolinecarbonitrile, 2-[[[(2S)-1-(6-benzothiazolylcarbonyl)-2-piperidinyl]methyl]amino]-6,7-difluoro- (CA INDEX NAME)

Absolute stereochemistry.



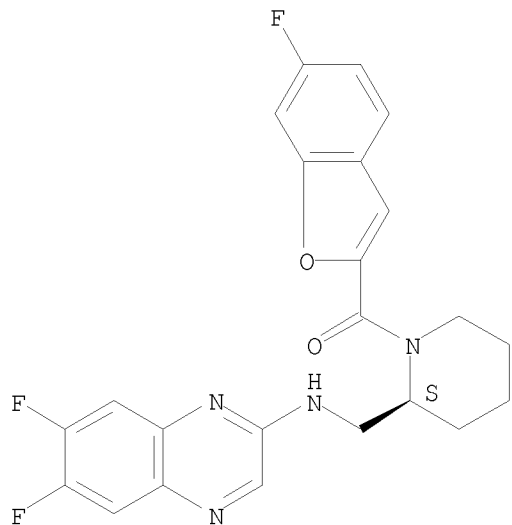
RN 475103-85-6 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl]-2-naphthalenyl- (CA INDEX NAME)

Absolute stereochemistry.



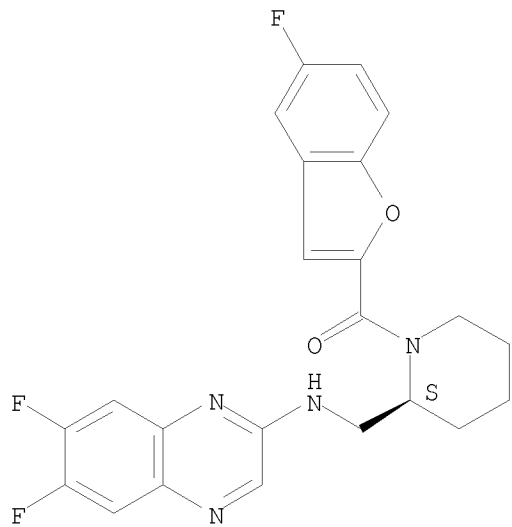
RN 475103-86-7 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl]-(6-fluoro-2-benzofuranyl)- (CA INDEX NAME)

Absolute stereochemistry.



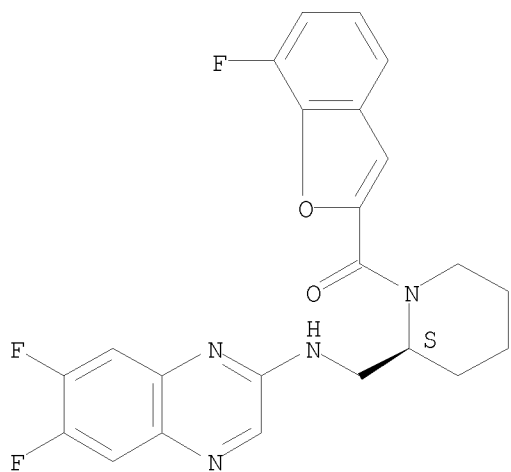
RN 475103-87-8 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl](5-fluoro-2-benzofuranyl)- (CA INDEX NAME)

Absolute stereochemistry.



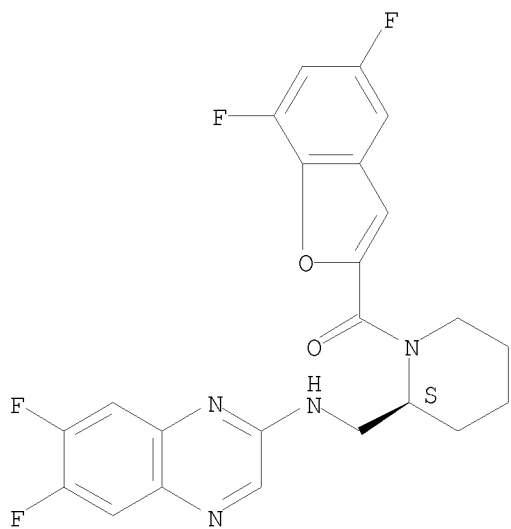
RN 475103-88-9 CAPLUS
 CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl](7-fluoro-2-benzofuranyl)- (CA INDEX NAME)

Absolute stereochemistry.



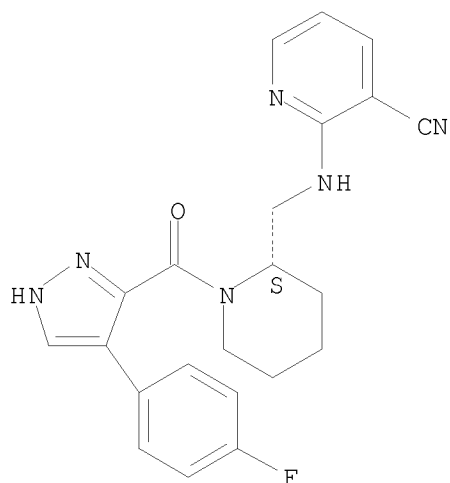
RN 475103-89-0 CAPLUS
 CN Methanone, (5,7-difluoro-2-benzofuranyl)[(2S)-2-[(6,7-difluoro-2-quinoxaliny)amino]methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-90-3 CAPLUS
 CN 3-Pyridinecarbonitrile, 2-[[[(2S)-1-[[4-(4-fluorophenyl)-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

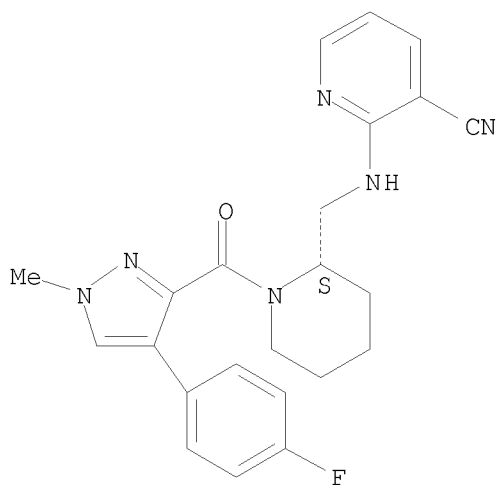
Absolute stereochemistry.



RN 475103-91-4 CAPLUS

CN 3-Pyridinecarbonitrile, 2-[[[(2S)-1-[[4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

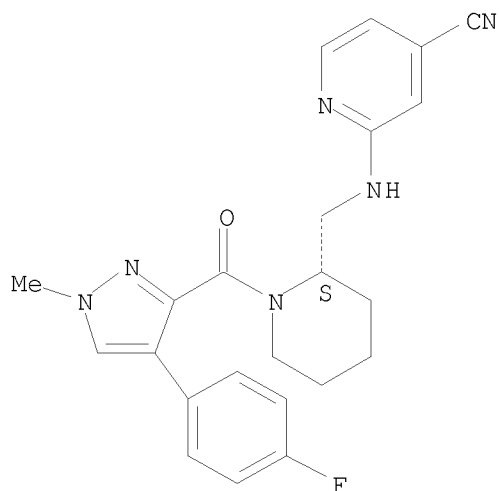
Absolute stereochemistry.



RN 475103-92-5 CAPLUS

CN 4-Pyridinecarbonitrile, 2-[[[(2S)-1-[[4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

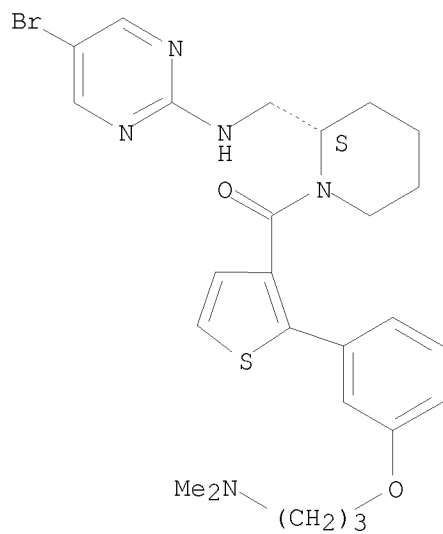
Absolute stereochemistry.



RN 475103-93-6 CAPLUS

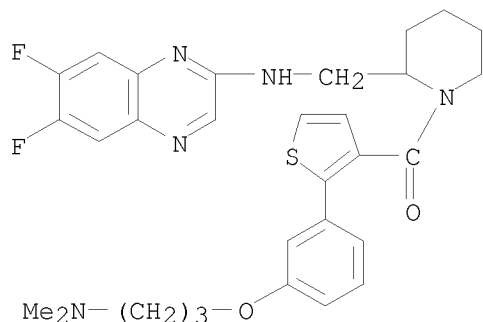
CN Methanone, [(2S)-2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl][2-[3-[3-(dimethylamino)propoxy]phenyl]-3-thienyl]- (CA INDEX NAME)

Absolute stereochemistry.



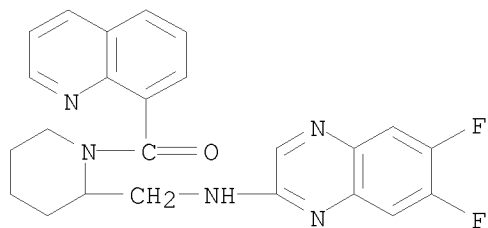
RN 475103-94-7 CAPLUS

CN Methanone, [2-[[(6,7-difluoro-2-quinoxaliny)amino]methyl]-1-piperidinyl][2-[3-[3-(dimethylamino)propoxy]phenyl]-3-thienyl]- (CA INDEX NAME)



RN 475103-95-8 CAPLUS

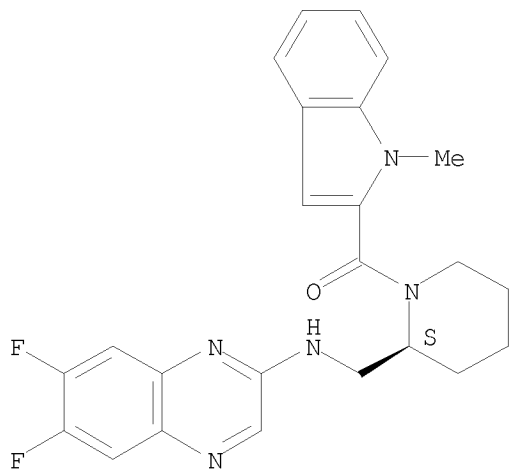
CN Methanone, [2-[[[(6,7-difluoro-2-quinoxalinyloxy)methyl]-1-piperidinyloxy]-8-quinolinyloxy]-1-methyl-4-phenylpiperidin-4-yl]-1-methyl-4-phenylpiperidin-4-ylmethanone (CA INDEX NAME)



RN 475103-96-9 CAPLUS

CN Methanone, [(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)methyl]-1-piperidinyloxy]-1-methyl-4-phenylpiperidin-4-yl]-1-methyl-4-phenylpiperidin-4-ylmethanone (CA INDEX NAME)

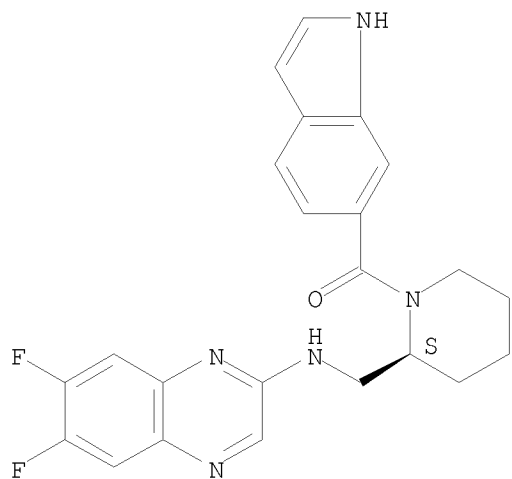
Absolute stereochemistry.



RN 475103-97-0 CAPLUS

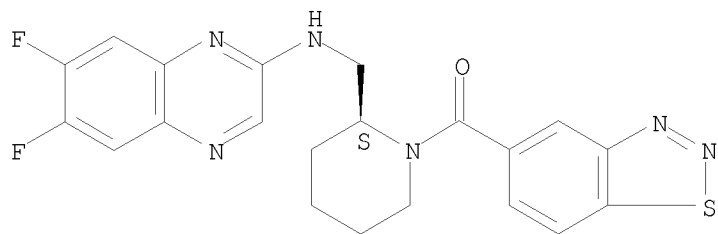
CN Methanone, [(2S)-2-[[[(6,7-difluoro-2-quinoxalinyloxy)methyl]-1-piperidinyloxy]-1-methyl-4-phenylpiperidin-4-yl]-1-methyl-4-phenylpiperidin-4-ylmethanone (CA INDEX NAME)

Absolute stereochemistry.



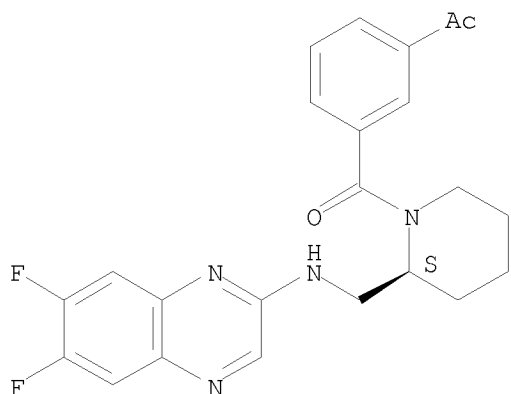
RN 475103-98-1 CAPLUS
 CN Methanone, 1,2,3-benzothiadiazol-5-yl[(2S)-2-[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyloxy- (CA INDEX NAME)

Absolute stereochemistry.



RN 475103-99-2 CAPLUS
 CN Ethanone, 1-[3-[[[(2S)-2-[[6,7-difluoro-2-quinoxalinyloxy]amino]methyl]-1-piperidinyloxy]carbonyl]phenyl]- (CA INDEX NAME)

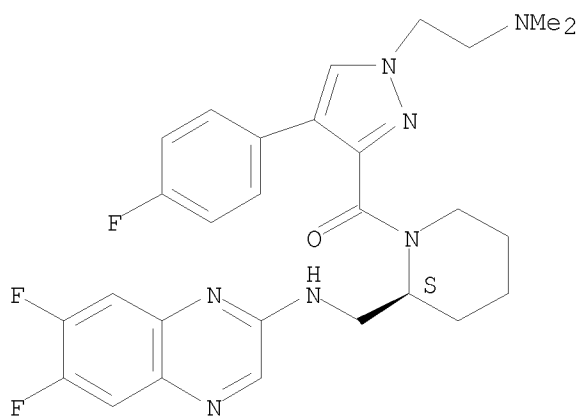
Absolute stereochemistry.



RN 475104-00-8 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidiny] [1-[2-(dimethylamino)ethyl]-4-(4-fluorophenyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

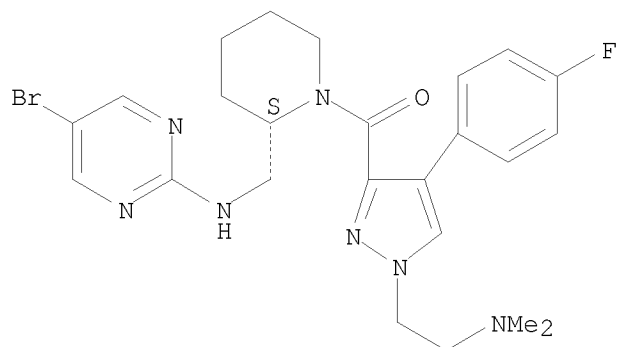
Absolute stereochemistry.



RN 475104-01-9 CAPLUS

CN Methanone, [(2S)-2-[[[5-bromo-2-pyrimidinyl]amino]methyl]-1-piperidiny] [1-[2-(dimethylamino)ethyl]-4-(4-fluorophenyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

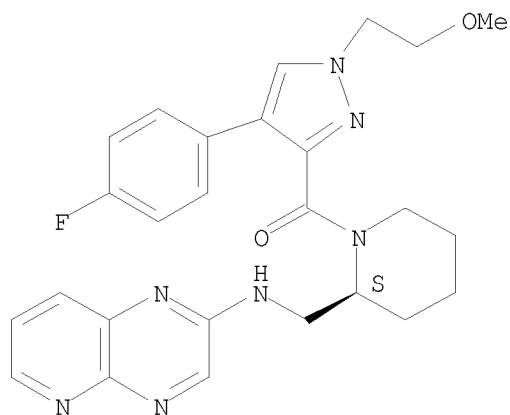
Absolute stereochemistry.



RN 475104-02-0 CAPLUS

CN Methanone, [4-(4-fluorophenyl)-1-(2-methoxyethyl)-1H-pyrazol-3-yl][(2S)-2-[(pyrido[2,3-b]pyrazin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

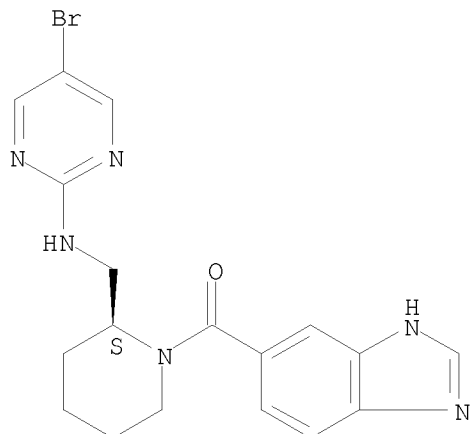
Absolute stereochemistry.



RN 475104-03-1 CAPLUS

CN Methanone, 1H-benzimidazol-6-yl[(2S)-2-[[5-bromo-2-pyrimidinyl)amino)methyl]-1-piperidinyl]- (CA INDEX NAME)

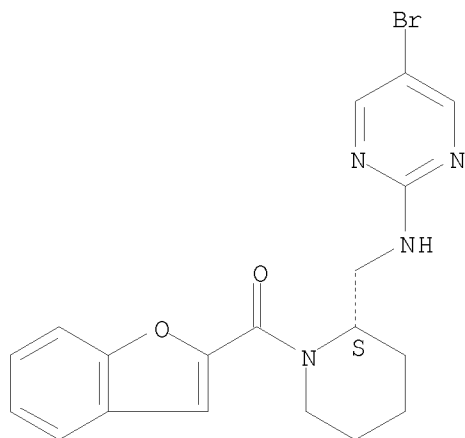
Absolute stereochemistry.



RN 475104-04-2 CAPLUS

CN Methanone, 2-benzofuranyl[(2S)-2-[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidiny]- (CA INDEX NAME)

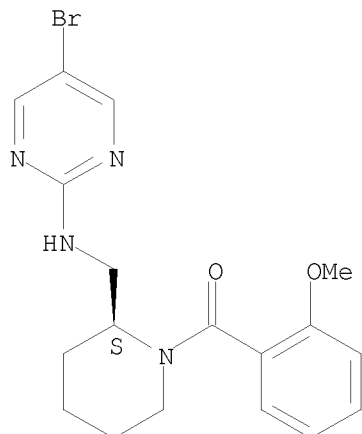
Absolute stereochemistry.



RN 475104-05-3 CAPLUS

CN Methanone, [(2S)-2-[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidiny] (2-methoxyphenyl)- (CA INDEX NAME)

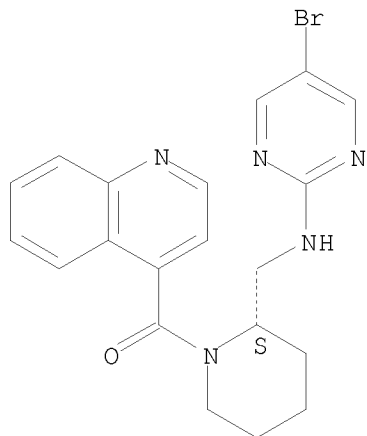
Absolute stereochemistry.



RN 475104-06-4 CAPLUS

CN Methanone, [(2S)-2-[[5-bromo-2-pyrimidinyl]amino]methyl]-1-piperidinyl]-4-quinolinyl- (CA INDEX NAME)

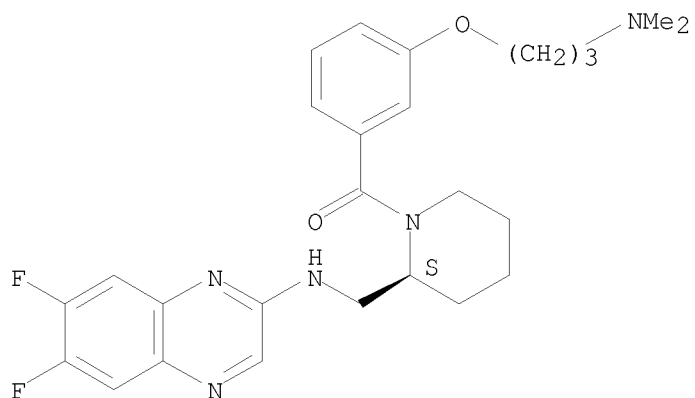
Absolute stereochemistry.



RN 475104-07-5 CAPLUS

CN Methanone, [(2S)-2-[[6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl]-3-[3-(dimethylamino)propoxy]phenyl- (CA INDEX NAME)

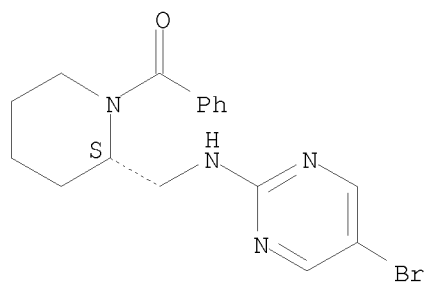
Absolute stereochemistry.



RN 475104-09-7 CAPLUS

CN Methanone, [(2S)-2-[[5-bromo-2-pyrimidinyl]amino]methyl]-1-piperidinyl]phenyl- (CA INDEX NAME)

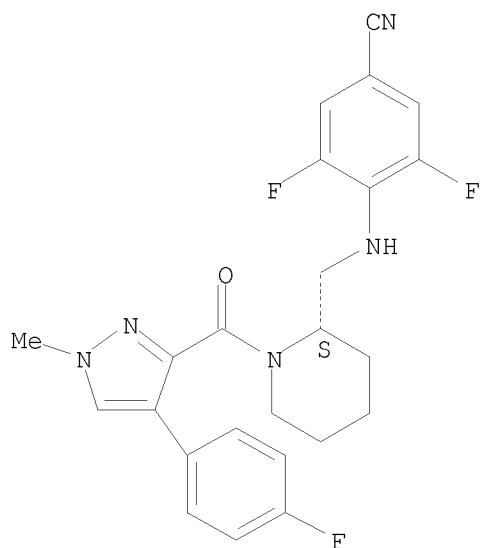
Absolute stereochemistry.



RN 475104-10-0 CAPLUS

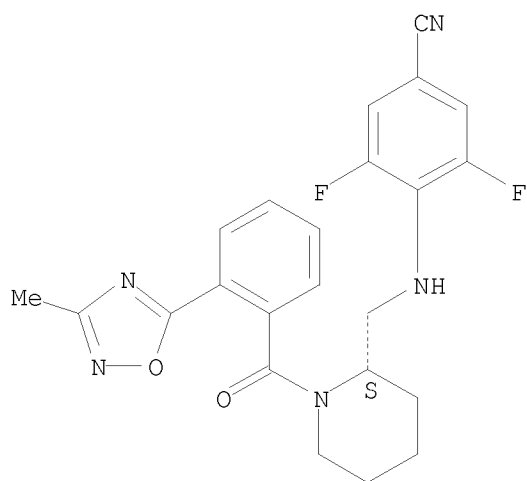
CN Benzonitrile, 3,5-difluoro-4-[[[(2S)-1-[[4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



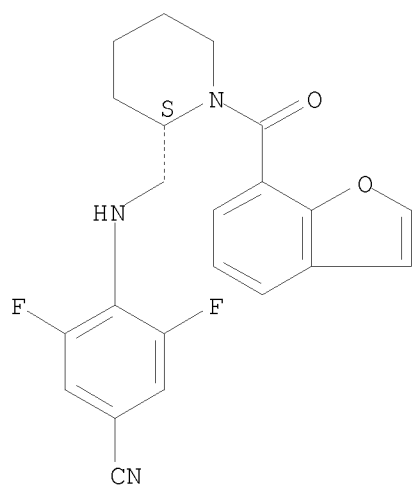
RN 475104-11-1 CAPLUS
 CN Benzonitrile, 3,5-difluoro-4-[[[(2S)-1-[2-(3-methyl-1,2,4-oxadiazol-5-yl)benzoyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.

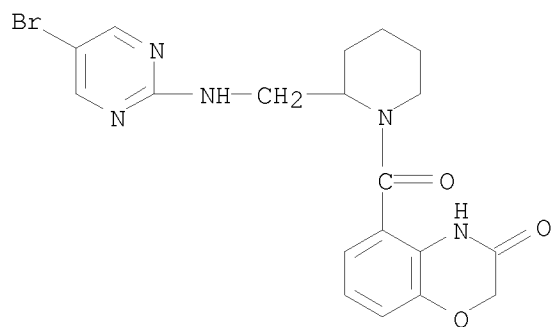


RN 475104-12-2 CAPLUS
 CN Benzonitrile, 4-[[[(2S)-1-(7-benzofuranylcarbonyl)-2-piperidinyl]methyl]amino]-3,5-difluoro- (CA INDEX NAME)

Absolute stereochemistry.

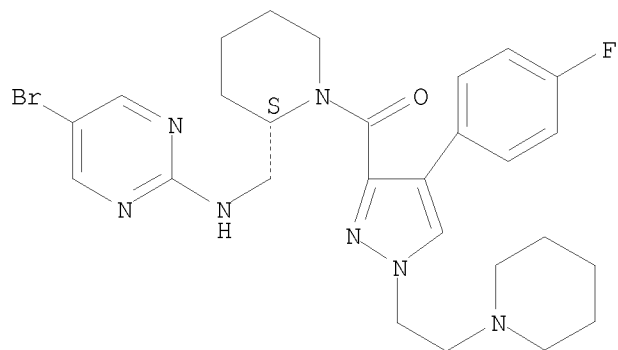


RN 475104-13-3 CAPLUS
 CN 2H-1,4-Benzoxazin-3(4H)-one, 5-[[2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidiny]carbonyl]-1-piperidiny]methyl]-4-fluorophenyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



RN 475104-14-4 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidiny][4-(4-fluorophenyl)-1-[2-(1-piperidiny)ethyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)

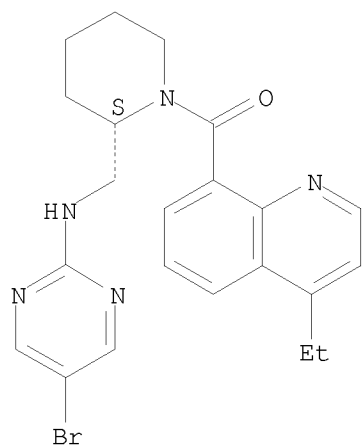
Absolute stereochemistry.



RN 475104-15-5 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl](4-ethyl-8-quinolinyl)- (CA INDEX NAME)

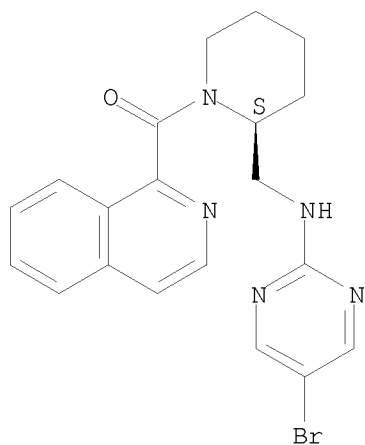
Absolute stereochemistry.



RN 475104-16-6 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl]-1-isoquinolinyl- (CA INDEX NAME)

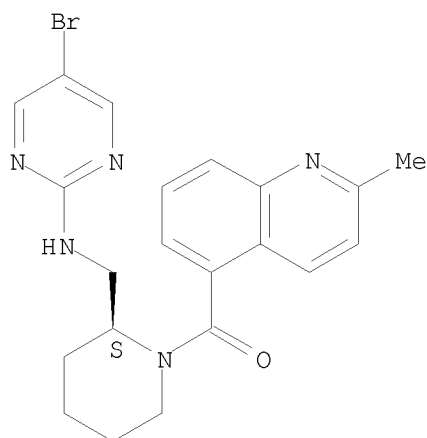
Absolute stereochemistry.



RN 475104-17-7 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl](2-methyl-5-quinolinyl)- (CA INDEX NAME)

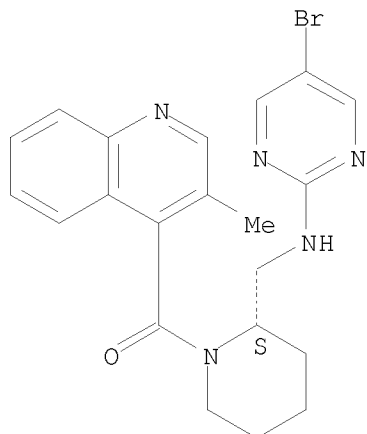
Absolute stereochemistry.



RN 475104-18-8 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl](3-methyl-4-quinolinyl)- (CA INDEX NAME)

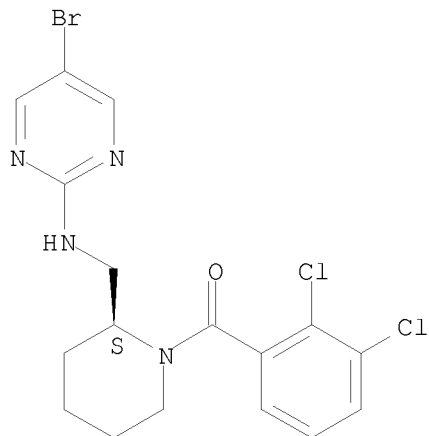
Absolute stereochemistry.



RN 475104-19-9 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl](2,3-dichlorophenyl)- (CA INDEX NAME)

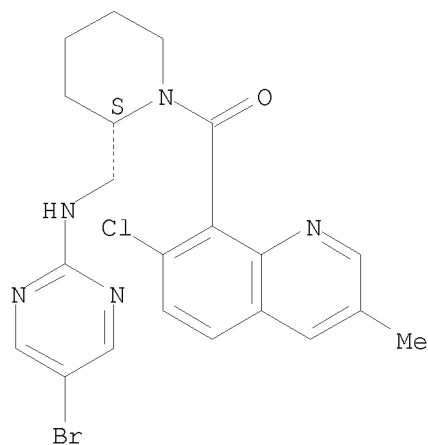
Absolute stereochemistry.



RN 475104-20-2 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl](7-chloro-3-methyl-8-quinolinyl)- (CA INDEX NAME)

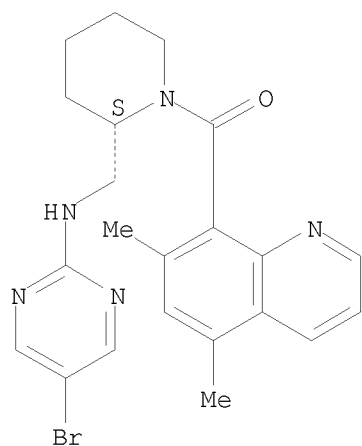
Absolute stereochemistry.



RN 475104-22-4 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl](5,7-dimethyl-8-quinolinyl)- (CA INDEX NAME)

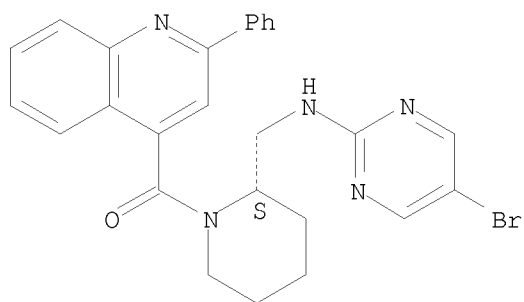
Absolute stereochemistry.



RN 475104-23-5 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl](2-phenyl-4-quinolinyl)- (CA INDEX NAME)

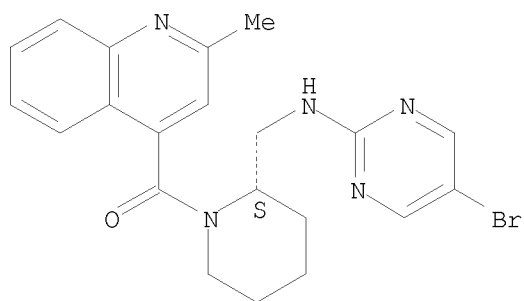
Absolute stereochemistry.



RN 475104-24-6 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl]] (2-methyl-4-quinolinyl)- (CA INDEX NAME)

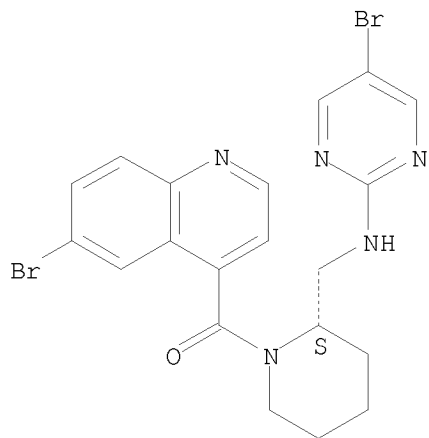
Absolute stereochemistry.



RN 475104-25-7 CAPLUS

CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl]] (6-bromo-4-quinolinyl)- (CA INDEX NAME)

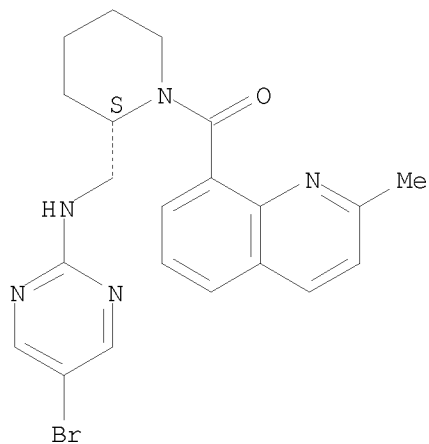
Absolute stereochemistry.



RN 475104-26-8 CAPLUS

CN Methanone, [(2S)-2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl] (2-methyl-8-quinolinyl)- (CA INDEX NAME)

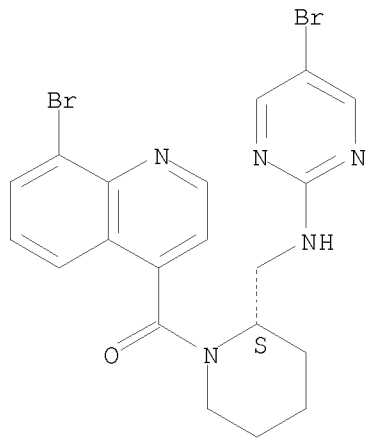
Absolute stereochemistry.



RN 475104-27-9 CAPLUS

CN Methanone, [(2S)-2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl] (8-bromo-4-quinolinyl)- (CA INDEX NAME)

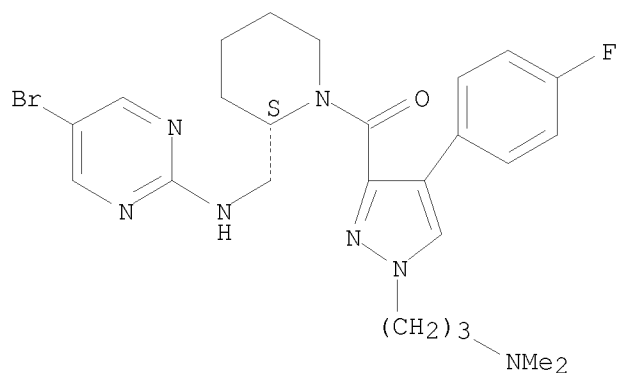
Absolute stereochemistry.



RN 475104-28-0 CAPLUS

CN Methanone, [(2S)-2-[[(5-bromo-2-pyrimidinyl)amino]methyl]-1-piperidinyl] [1-[3-(dimethylamino)propyl]-4-(4-fluorophenyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

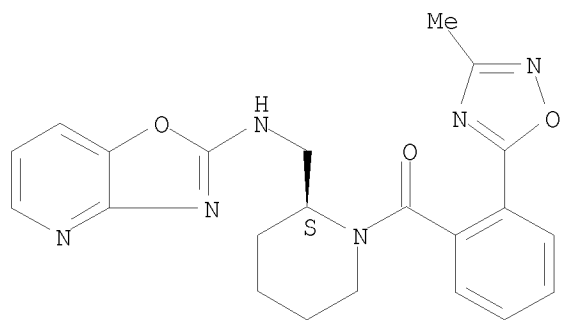
Absolute stereochemistry.



RN 475104-91-7 CAPLUS

CN Methanone, [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl][(2S)-2-[(oxazolo[4,5-b]pyridin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

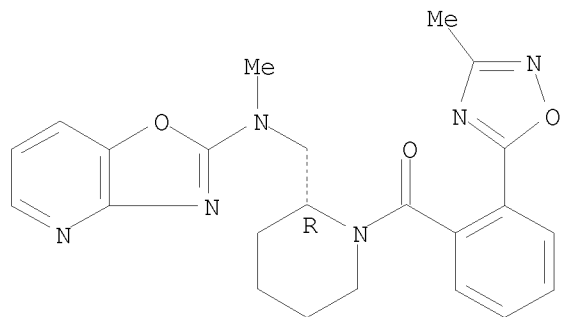
Absolute stereochemistry.



RN 475104-92-8 CAPLUS

CN Methanone, [2-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl][(2R)-2-[(methyloxazolo[4,5-b]pyridin-2-ylamino)methyl]-1-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.

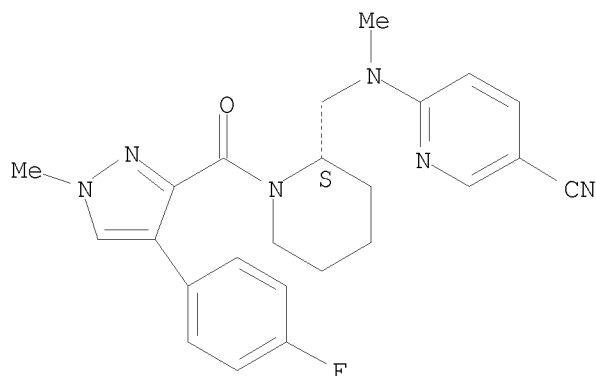


RN 475104-93-9 CAPLUS

CN 3-Pyridinecarbonitrile, 6-[[[(2S)-1-[[4-(4-fluorophenyl)-1-methyl-1H-

pyrazol-3-yl]carbonyl]-2-piperidinyl)methyl)methylamino]- (CA INDEX NAME)

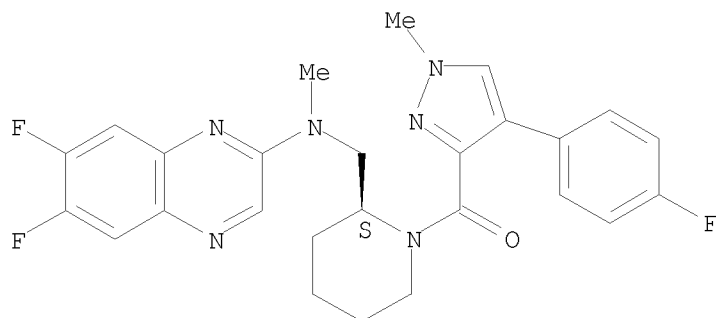
Absolute stereochemistry.



RN 475104-94-0 CAPLUS

CN Methanone, [(2S)-2-[[[6,7-difluoro-2-quinoxaliny]methylamino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (CA INDEX NAME)

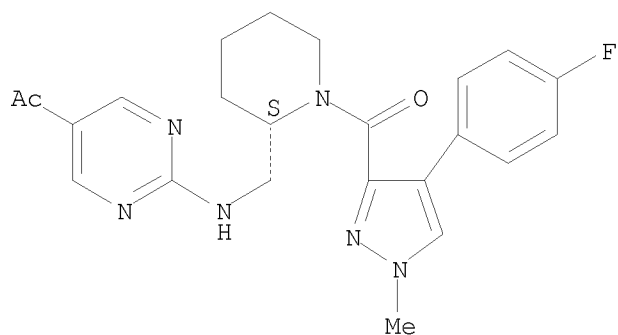
Absolute stereochemistry.



RN 475104-95-1 CAPLUS

CN Ethanone, 1-[2-[[[(2S)-1-[[4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl)methyl]amino]-5-pyrimidinyl]- (CA INDEX NAME)

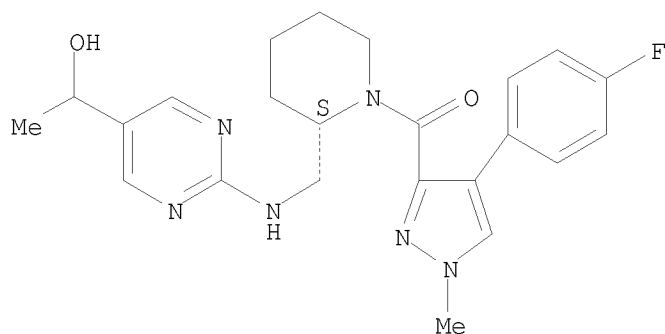
Absolute stereochemistry.



RN 475104-96-2 CAPLUS

CN Methanone, [4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl][(2S)-2-[[[5-(1-hydroxyethyl)-2-pyrimidinyl]amino]methyl]-1-piperidinyl]- (CA INDEX NAME)

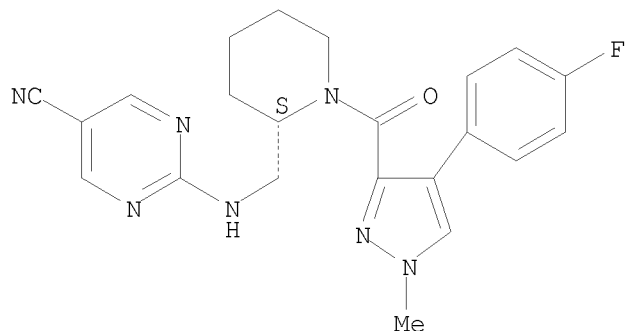
Absolute stereochemistry.



RN 475104-97-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[[[(2S)-1-[[4-(4-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.

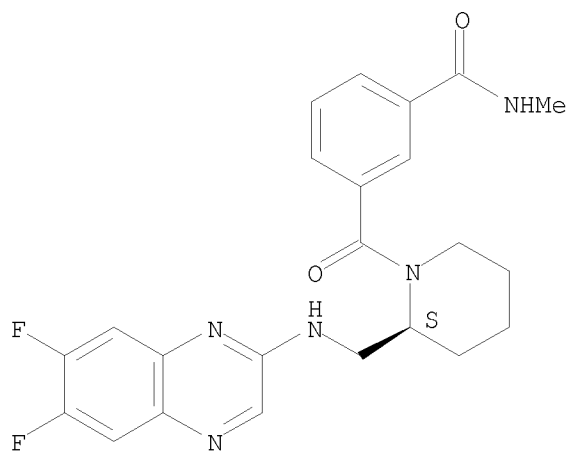


RN 475104-98-4 CAPLUS

CN Benzamide, 3-[[[(2S)-2-[[[(6,7-difluoro-2-quinoxaliny]amino]methyl]-1-

piperidinyl]carbonyl]-N-methyl- (CA INDEX NAME)

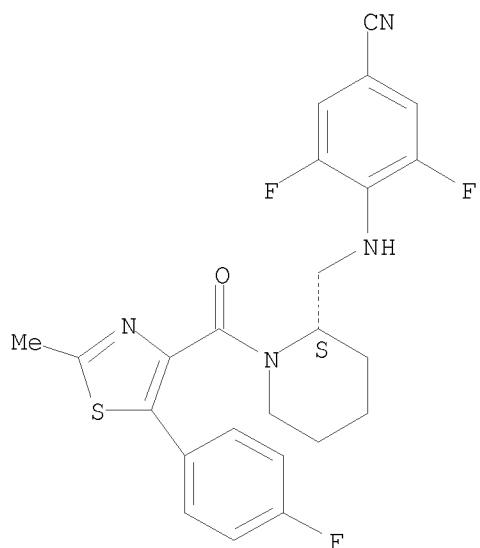
Absolute stereochemistry.



RN 475105-05-6 CAPLUS

CN Benzonitrile, 3,5-difluoro-4-[[[(2S)-1-[[5-(4-fluorophenyl)-2-methyl-4-thiazolyl]carbonyl]-2-piperidinyl]methyl]amino]- (CA INDEX NAME)

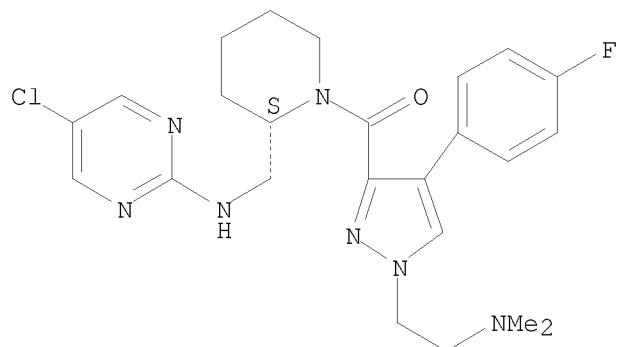
Absolute stereochemistry.



RN 475105-23-8 CAPLUS

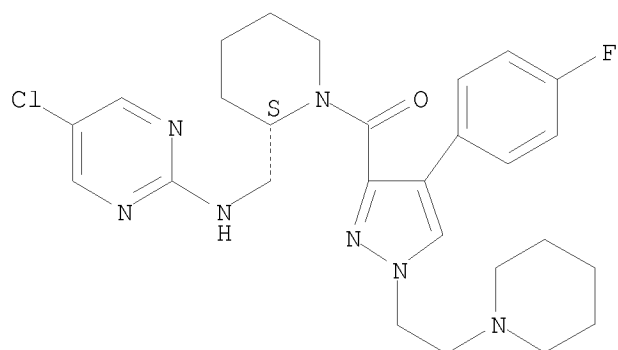
CN Methanone, [(2S)-2-[[[(5-chloro-2-pyrimidinyl)amino]methyl]-1-piperidinyl][1-[2-(dimethylamino)ethyl]-4-(4-fluorophenyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



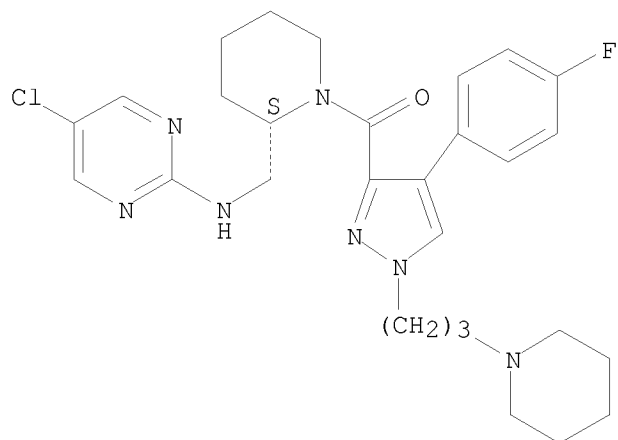
RN 475105-24-9 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-chloro-2-pyrimidinyl)amino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-[2-(1-piperidinyl)ethyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



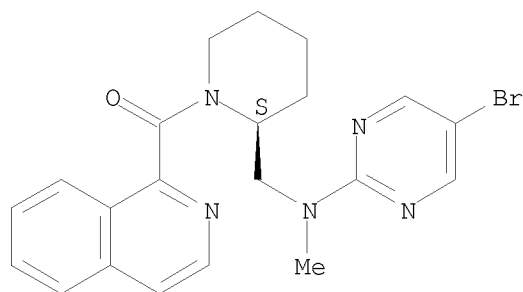
RN 475105-25-0 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-chloro-2-pyrimidinyl)amino]methyl]-1-piperidinyl][4-(4-fluorophenyl)-1-[3-(1-piperidinyl)propyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



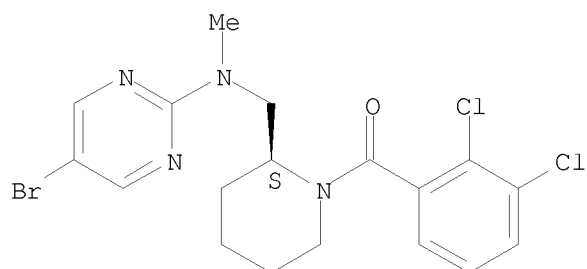
RN 475105-26-1 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)methylamino]methyl]-1-piperidinyl]-1-isoquinolinyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 475105-27-2 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-bromo-2-pyrimidinyl)methylamino]methyl]-1-piperidinyl](2,3-dichlorophenyl)- (CA INDEX NAME)

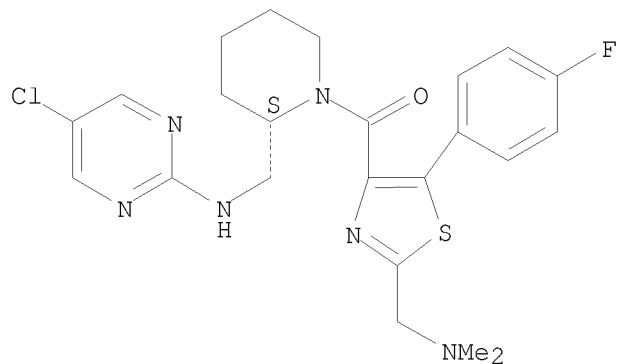
Absolute stereochemistry.



RN 475105-28-3 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-chloro-2-pyrimidinyl)amino]methyl]-1-

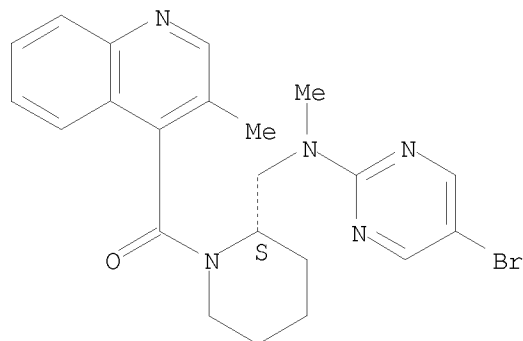
piperidinyl][2-[(dimethylamino)methyl]-5-(4-fluorophenyl)-4-thiazolyl]-
(CA INDEX NAME)

Absolute stereochemistry.



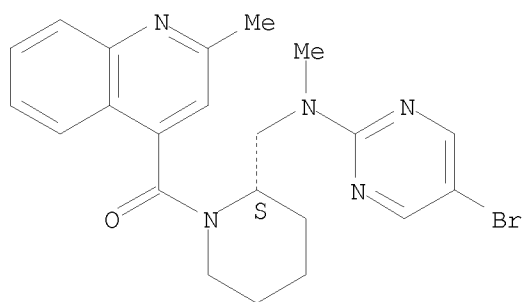
RN 475105-29-4 CAPLUS
CN Methanone, [(2S)-2-[[(5-bromo-2-pyrimidinyl)methylamino]methyl]-1-
piperidinyl](3-methyl-4-quinolinyl)- (CA INDEX NAME)

Absolute stereochemistry.



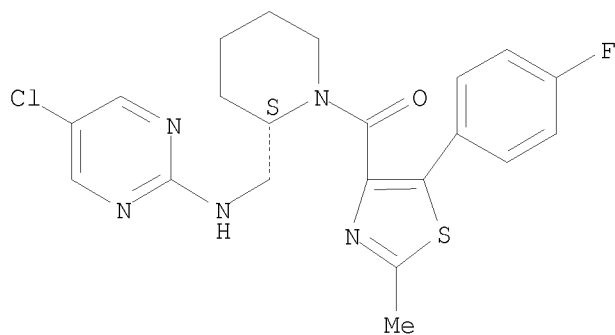
RN 475105-30-7 CAPLUS
CN Methanone, [(2S)-2-[[(5-bromo-2-pyrimidinyl)methylamino]methyl]-1-
piperidinyl](2-methyl-4-quinolinyl)- (CA INDEX NAME)

Absolute stereochemistry.



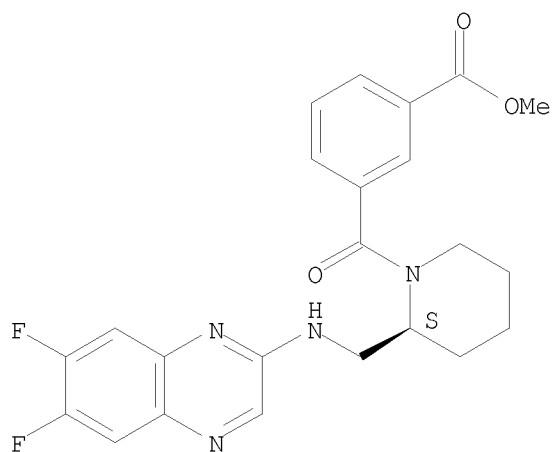
RN 475105-31-8 CAPLUS
 CN Methanone, [(2S)-2-[[[(5-chloro-2-pyrimidinyl)amino]methyl]-1-piperidinyl][5-(4-fluorophenyl)-2-methyl-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.



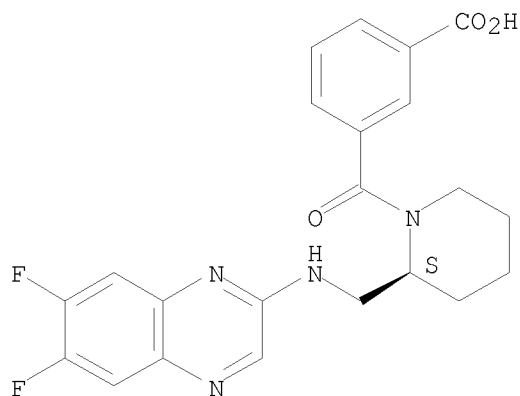
IT 475106-45-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of N-aroyl cyclic amines as orexin antagonists)
 RN 475106-45-7 CAPLUS
 CN Benzoic acid, 3-[[[(2S)-2-[[[(6,7-difluoro-2-quinoxaliny]amino]methyl]-1-piperidinyl]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



IT 475106-11-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of N-aroyl cyclic amines as orexin antagonists)
 RN 475106-11-7 CAPLUS
 CN Benzoic acid, 3-[[[(2S)-2-[[[(6,7-difluoro-2-quinoxaliny)amino]methyl]-1-
 piperidinyl]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

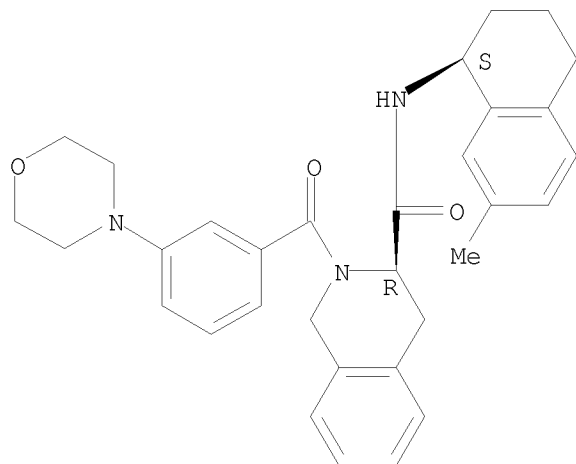
L4 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:554265 CAPLUS
 DOCUMENT NUMBER: 137:243205
 TITLE: Comparison of the computer programs DEREK and TOPKAT
 to predict bacterial mutagenicity
 AUTHOR(S): Cariello, Neal F.; Wilson, John D.; Britt, Ben H.;
 Wedd, David J.; Burlinson, Brian; Gombar, Vijay
 CORPORATE SOURCE: Safety Assessment, GlaxoSmithKline Inc., Research
 Triangle Park, NC, 27709, USA

SOURCE: Mutagenesis (2002), 17(4), 321-329
CODEN: MUTAEX; ISSN: 0267-8357
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The performance of two computer programs, DEREK and TOPKAT, was examined with regard to predicting the outcome of the Ames bacterial mutagenicity assay. The results of over 400 Ames tests conducted at Glaxo Wellcome (now GlaxoSmithKline) during the last 15 yr on a wide variety of chemical classes were compared with the mutagenicity predictions of both computer programs. DEREK was considered concordant with the Ames assay if (i) the Ames assay was neg. (not mutagenic) and no structural alerts for mutagenicity were identified or (ii) the Ames assay was pos. (mutagenic) and at least one structural alert was identified. Conversely, the DEREK output was considered discordant if (i) the Ames assay was neg. and any structural alert was identified or (ii) the Ames assay was pos. and no structural alert was identified. The overall concordance of the DEREK program with the Ames results was 65% and the overall discordance was 35%, based on over 400 compds. About 23% of the test mols. were outside the permissible limits of the optimum prediction space of TOPKAT. Another 4% of the compds. were either not processable or had indeterminate mutagenicity predictions; these mols. were excluded from the TOPKAT anal. If the TOPKAT probability was (i) ≥ 0.7 the mol. was predicted to be mutagenic, (ii) ≤ 0.3 the compound was predicted to be non-mutagenic and (iii) between 0.3 and 0.7 the prediction was considered indeterminate. From over 300 acceptable predictions, the overall TOPKAT concordance was 73% and the overall discordance was 27%. While the overall concordance of the TOPKAT program was higher than DEREK, TOPKAT fared more poorly than DEREK in the critical Ames-pos. category, where 60% of the compds. were incorrectly predicted by TOPKAT as neg. but were mutagenic in the Ames test. For DEREK, 54% of the Ames-pos. mols. had no structural alerts and were predicted to be non-mutagenic. Alternative methods of analyzing the output of the programs to increase the accuracy with Ames-pos. compds. are discussed.

IT 461053-64-5
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(computer programs DEREK and TOPKAT to predict bacterial mutagenicity)
RN 461053-64-5 CAPLUS
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
N-[(1S)-1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl]-, (3R)- (CA INDEX
NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:336726 CAPLUS

DOCUMENT NUMBER: 138:147163

TITLE: CCK2 receptor antagonists containing the conformationally constrained phenylalanine derivatives, including the new amino acid Xic
AUTHOR(S): Gibson, Susan E.; Guillo, Nathalie; Jones, Jerome O.; Buck, Ildiko M.; Kalindjian, S. Barret; Roberts, Sonia; Tozer, Matthew J.

CORPORATE SOURCE: Department of Chemistry, King's College London, Strand, London, WC2R 2LS, UK

SOURCE: European Journal of Medicinal Chemistry (2002), 37(5), 379-389

CODEN: EJMC A5; ISSN: 0223-5234

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:147163

AB The conformationally constrained analogs of phenylalanine, tetrahydroisoquinoline-3-carboxylic acid (Tic), Sic, Hic and Nic, and the new amino acid Xic have been incorporated into a potent and highly selective cholecystokinin-2 (CCK2) receptor antagonist (2) in place of the phenylalanine residue, producing a group of compds. High selectivities for CCK2 over CCK1 were observed for compds. The in vitro profile of the analog containing the Nic residue (15d) was identical to that of one compound, whereas the alternative conformational constraints resulted in a significant loss of affinity. The apparent advantage of Nic in the context of these CCK2 ligands was subsequently demonstrated to be statistically significant.

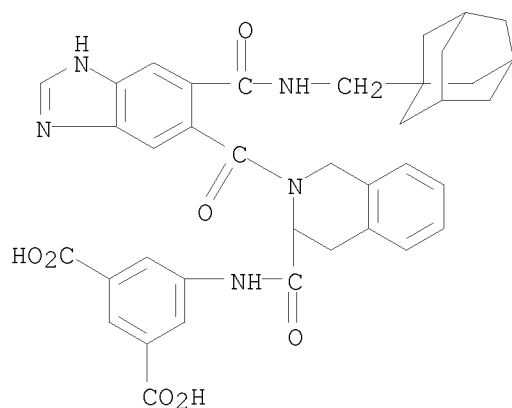
IT 192134-02-4P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(CCK2 receptor antagonists containing the conformationally constrained phenylalanine derivs., including the new amino acid Xic)

RN 192134-02-4 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[[[1,2,3,4-tetrahydro-2-[[5-
[[(tricyclo[3.3.1.1^{3,7}]dec-1-ylmethyl)amino]carbonyl]-1H-benzimidazol-6-
yl]carbonyl]-3-isoquinolinyl]carbonyl]amino]- (CA INDEX NAME)

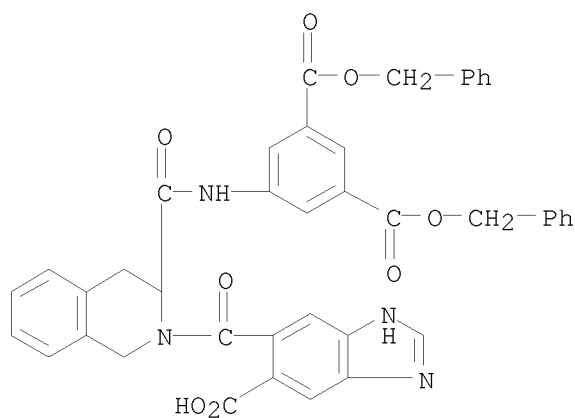


IT 192133-93-0P 192133-97-4P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(CCK2 receptor antagonists containing the conformationally constrained
phenylalanine derivs., including the new amino acid Xic)

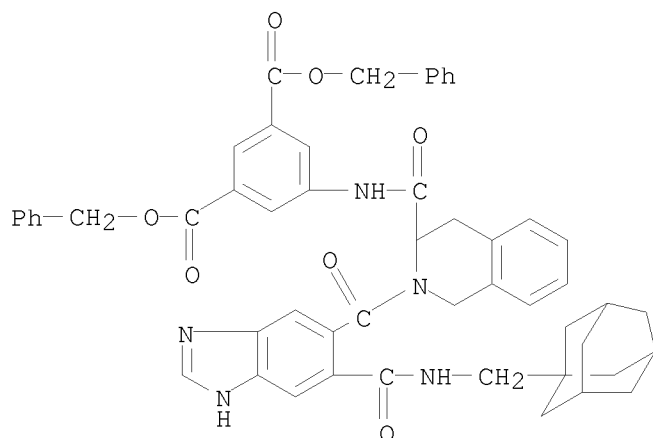
RN 192133-93-0 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[[[2-[(6-carboxy-1H-benzimidazol-5-
yl)carbonyl]-1,2,3,4-tetrahydro-3-isoquinolinyl]carbonyl]amino]-,
1,3-bis(phenylmethyl) ester (CA INDEX NAME)



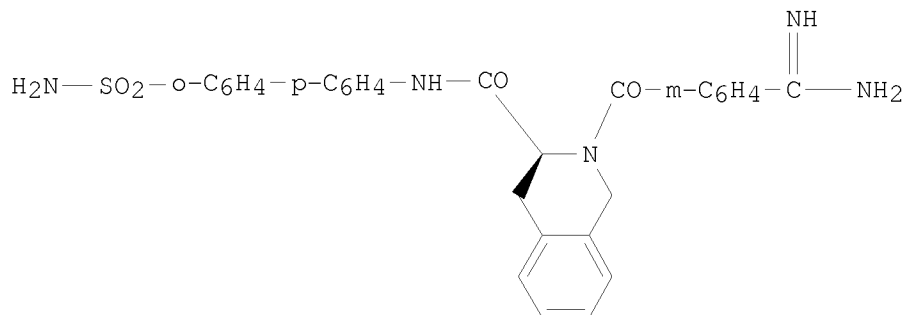
RN 192133-97-4 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[[[1,2,3,4-tetrahydro-2-[[5-
[[(tricyclo[3.3.1.1^{3,7}]dec-1-ylmethyl)amino]carbonyl]-1H-benzimidazol-6-
yl]carbonyl]-3-isoquinolinyl]carbonyl]amino]-, 1,3-bis(phenylmethyl) ester
(CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:780023 CAPLUS
 DOCUMENT NUMBER: 136:184072
 TITLE: Design, Synthesis, and SAR of Amino Acid Derivatives as Factor Xa Inhibitors
 AUTHOR(S): Su, Ting; Wu, Yanhong; Doughan, Brandon; Jia, Zhaozhong J.; Woolfrey, John; Huang, Brian; Wong, Paul; Park, Gary; Sinha, Uma; Scarborough, Robert M.; Zhu, Bing-yan
 CORPORATE SOURCE: COR Therapeutics, Inc., South San Francisco, CA, 94080, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(22), 2947-2950
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:184072
 GI



I

AB A series of potent and selective factor Xa inhibitors was synthesized

using various readily available amino acids as central templates. The most potent compound (I) displays IC₅₀ of 3 nM.

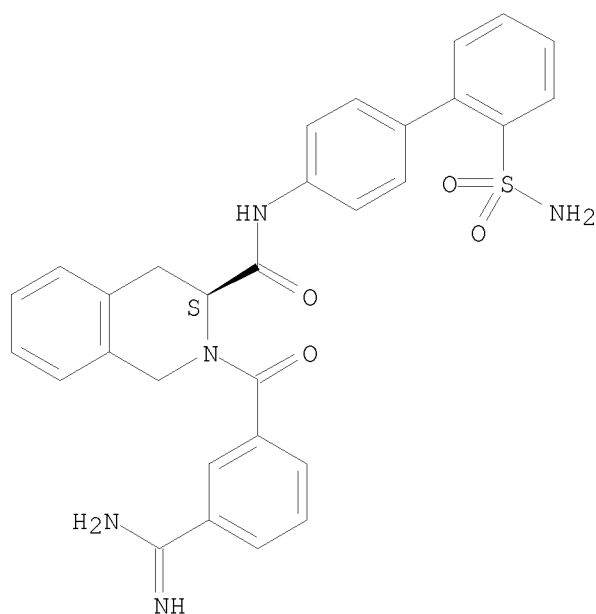
IT 398477-14-0P 398477-15-1P 398477-16-2P
398477-17-3P 398477-21-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. activity of amino acid benzamidine derivs. as Factor Xa inhibitors)

RN 398477-14-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(aminoiminomethyl)benzoyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

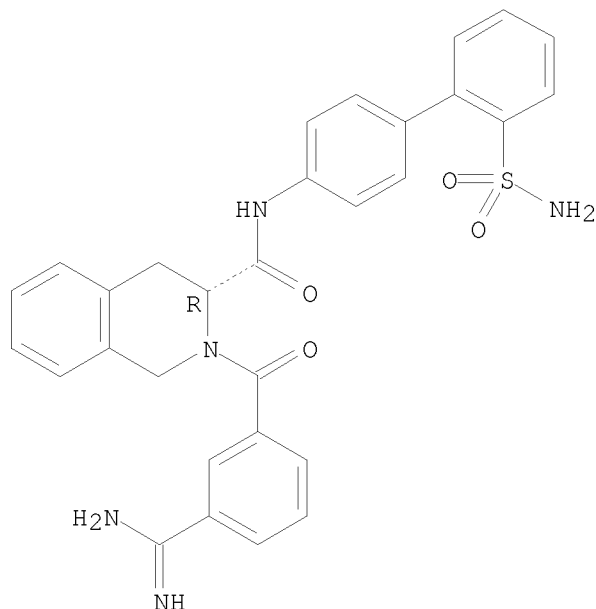
Absolute stereochemistry.



RN 398477-15-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(aminoiminomethyl)benzoyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-, (3R)- (CA INDEX NAME)

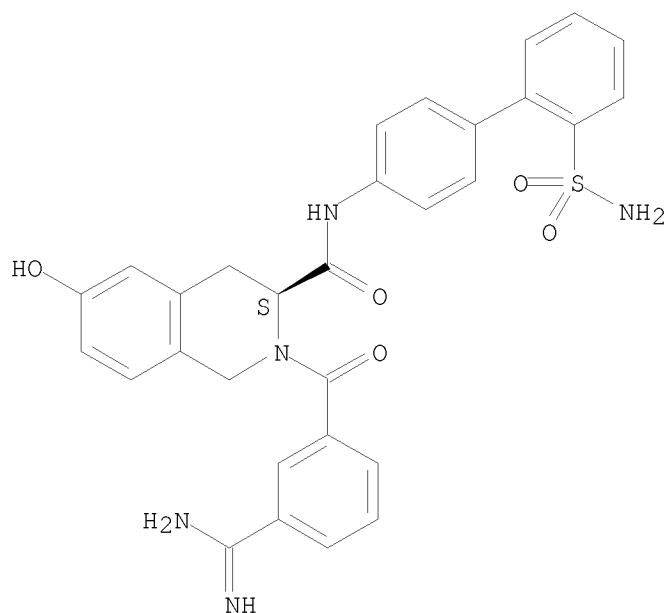
Absolute stereochemistry.



RN 398477-16-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(aminoiminomethyl)benzoyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-6-hydroxy-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.

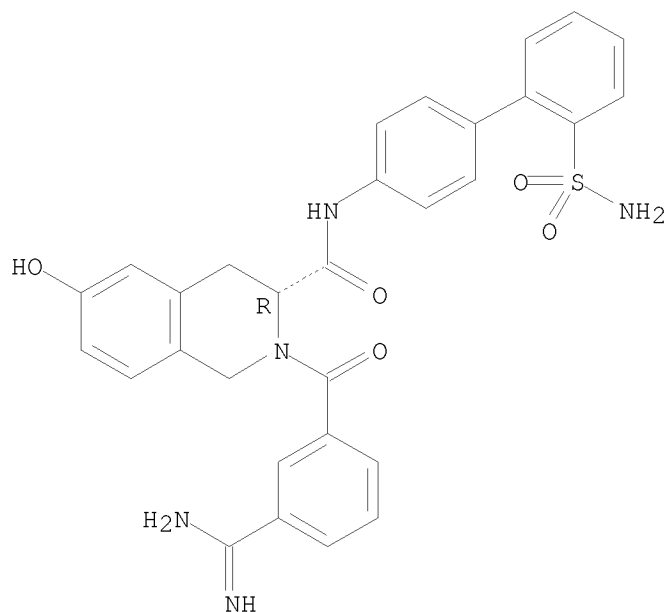


RN 398477-17-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(aminoiminomethyl)benzoyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-6-hydroxy-, (3R)-

(CA INDEX NAME)

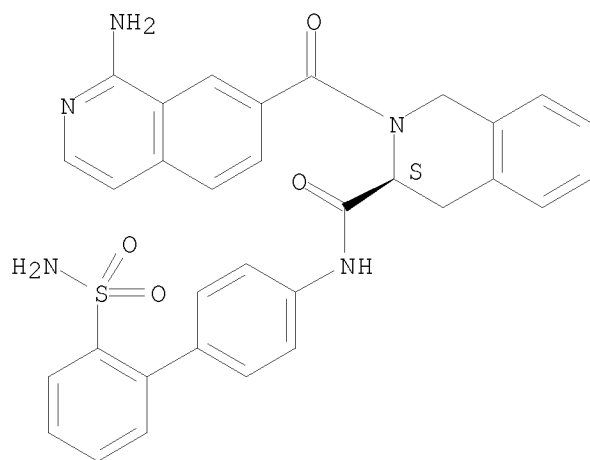
Absolute stereochemistry.



RN 398477-21-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[(1-amino-7-isoquinolinyl)carbonyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 398477-00-4P 398477-01-5P 398477-02-6P

398477-03-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

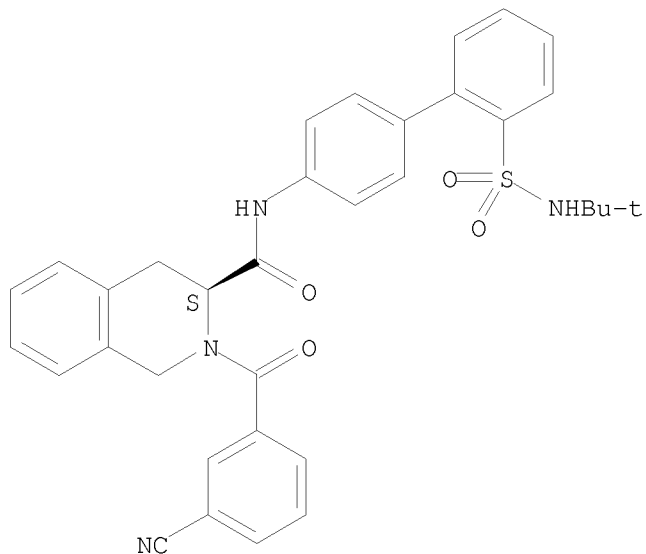
(preparation and biol. activity of amino acid benzamidine derivs. as Factor

Xa inhibitors)

RN 398477-00-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-cyanobenzoyl)-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-, (3S)- (CA INDEX NAME)

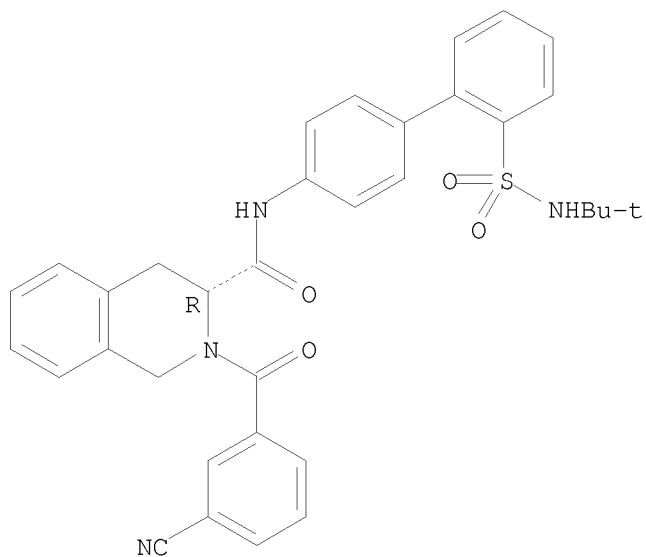
Absolute stereochemistry.



RN 398477-01-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-cyanobenzoyl)-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-, (3R)- (CA INDEX NAME)

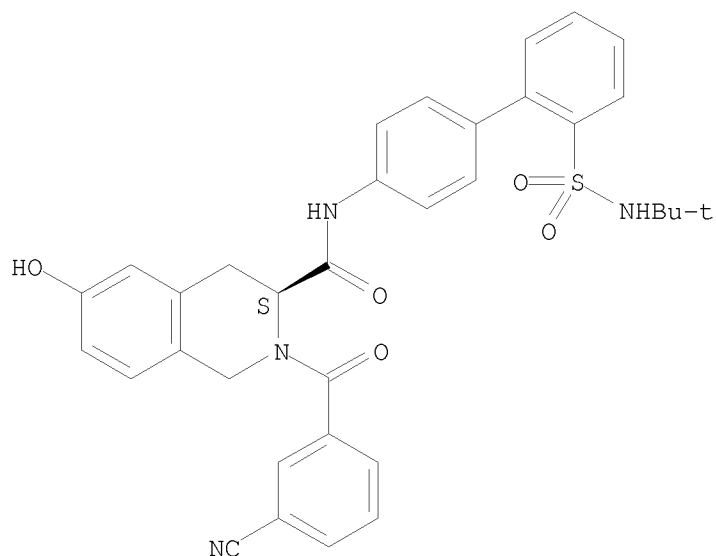
Absolute stereochemistry.



RN 398477-02-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-cyanobenzoyl)-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-6-hydroxy-, (3S)- (CA INDEX NAME)

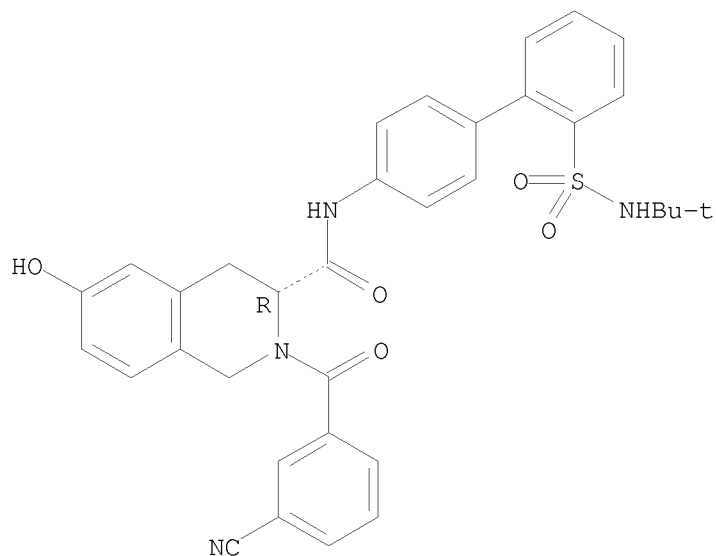
Absolute stereochemistry.



RN 398477-03-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(3-cyanobenzoyl)-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1,2,3,4-tetrahydro-6-hydroxy-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:117043 CAPLUS
 DOCUMENT NUMBER: 132:151680
 TITLE: Preparation of carbazoles, isoquinolines, indoles, and related compounds as follicle stimulating hormone mimetics for the treatment of infertility.
 INVENTOR(S): El Tayer, Nabil; Reddy, Adulla; Buckler, David; Magar, Sharad
 PATENT ASSIGNEE(S): Applied Research Systems Ars Holding N. V., Neth. Antilles
 SOURCE: PCT Int. Appl., 62 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000008015	A2	20000217	WO 1999-US17755	19990805
WO 2000008015	A3	20000511		
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2339018	A1	20000217	CA 1999-2339018	19990805
AU 9953931	A	20000228	AU 1999-53931	19990805
AU 772373	B2	20040422		
US 6235755	B1	20010522	US 1999-369222	19990805
EP 1102763	A2	20010530	EP 1999-939686	19990805
EP 1102763	B1	20041013		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002522433	T	20020723	JP 2000-563648	19990805
EP 1380582	A1	20040114	EP 2003-23514	19990805
EP 1380582	B1	20060614		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY			
AT 279407	T	20041015	AT 1999-939686	19990805
PT 1102763	T	20050131	PT 1999-939686	19990805
ES 2228084	T3	20050401	ES 1999-939686	19990805
IL 141063	A	20050619	IL 1999-141063	19990805
AT 329911	T	20060715	AT 2003-23514	19990805
ES 2261844	T3	20061116	ES 2003-23514	19990805
PT 1380582	T	20060831	PT 2003-23514	19990808
US 6423723	B1	20020723	US 2000-723495	20001128
US 20020147345	A1	20021010	US 2002-156431	20020528
US 6653338	B2	20031125		
AU 2004202858	A1	20040722	AU 2004-202858	20040625
AU 2004202858	B2	20060706		
PRIORITY APPLN. INFO.:			US 1998-95712P	P 19980807

AU 1999-53931	A3 19990805
EP 1999-939686	A3 19990805
US 1999-369222	A3 19990805
WO 1999-US17755	W 19990805
US 2000-723495	A3 20001128

OTHER SOURCE(S): MARPAT 132:151680

AB R5ZYR4XR3WNR1R2 [R1, R3, R4, R5 = H, (substituted) alkyl, alkenyl, alkynyl, alkoxy, alkoxy carbonyl, thioalkyl, acyl, acyloxy, aryl, cycloalkyl, heterocyclyl; R2 = H, (substituted) cycloalkyl, heterocyclyl, aryl, heteroaryl; NR1R2 = (substituted) heterocyclyl, heteroaryl; W = CO, NHCO, NHCOCH2, C:NH, CS, SO2, (substituted) CH2; X, Y = CH, N; Z = CO, NH, C:N, SO2, CONH], were prepared. Thus, 1-[(2-oxo-6-pentyl-2H-pyran)-3-carbonyl]piperidine-2-carboxylic acid 3-(9-ethylcarbazolyl)amide (prepared from BOC-Pro-OH, 3-amino-9-ethylcarbazole, and 2-oxo-6-pentyl-2H-pyran-3-carboxylic acid) stimulated estradiol production in the rat granulosa cell assay with EC50 = 1.4 μ M.

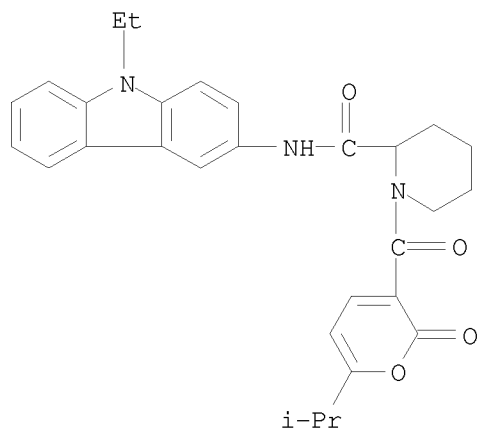
IT 258277-66-6P 258277-67-7P 258277-68-8P
 258277-80-4P 258277-82-6P 258277-83-7P
 258277-88-2P 258277-98-4P 258277-99-5P
 258278-02-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of carbazoles, isoquinolines, indoles, and related compds. as FSH mimetics for the treatment of infertility)

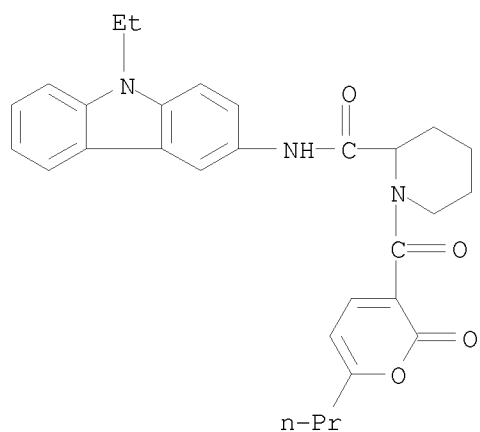
RN 258277-66-6 CAPLUS

CN 2-Piperidinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1-[[6-(1-methylethyl)-2-oxo-2H-pyran-3-yl]carbonyl]- (CA INDEX NAME)

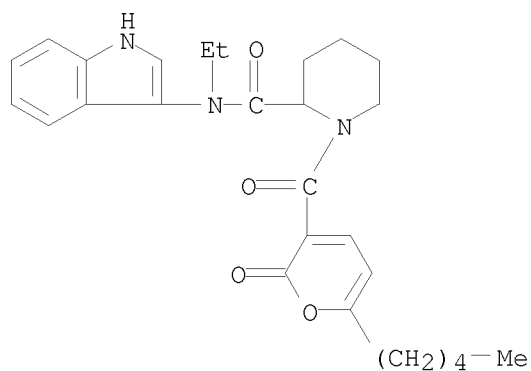


RN 258277-67-7 CAPLUS

CN 2-Piperidinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1-[(2-oxo-6-propyl-2H-pyran-3-yl)carbonyl]- (CA INDEX NAME)

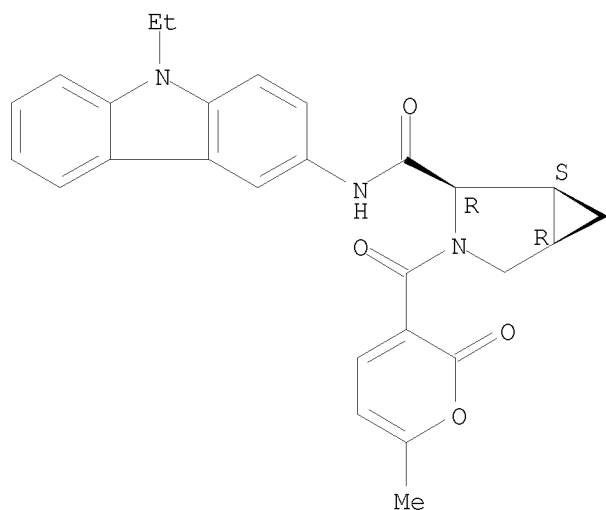


RN 258277-68-8 CAPLUS
 CN 2-Piperidinecarboxamide, N-ethyl-N-1H-indol-3-yl-1-[(2-oxo-6-pentyl-2H-pyran-3-yl)carbonyl]- (CA INDEX NAME)



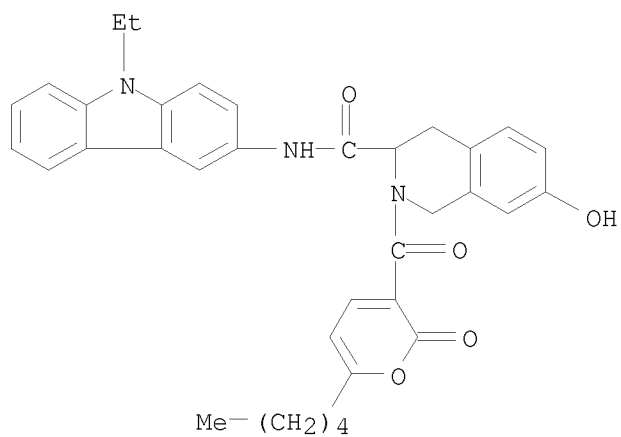
RN 258277-80-4 CAPLUS
 CN 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-(9-ethyl-9H-carbazol-3-yl)-3-[(6-methyl-2-oxo-2H-pyran-3-yl)carbonyl]-, (1R,2S,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



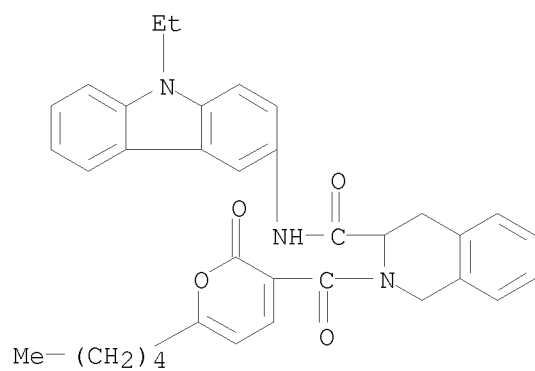
RN 258277-82-6 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1,2,3,4-tetrahydro-7-hydroxy-2-[(2-oxo-6-pentyl-2H-pyran-3-yl)carbonyl]- (CA INDEX NAME)



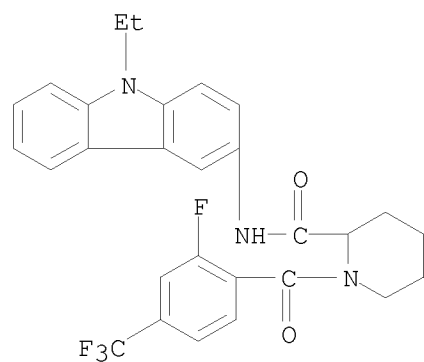
RN 258277-83-7 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1,2,3,4-tetrahydro-2-[(2-oxo-6-pentyl-2H-pyran-3-yl)carbonyl]- (CA INDEX NAME)



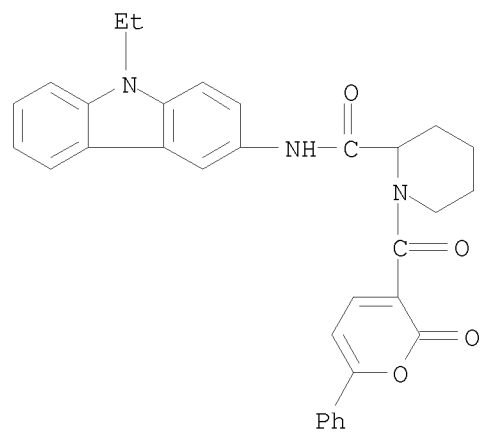
RN 258277-88-2 CAPLUS

CN 2-Piperidinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1-[2-fluoro-4-(trifluoromethyl)benzoyl]- (CA INDEX NAME)

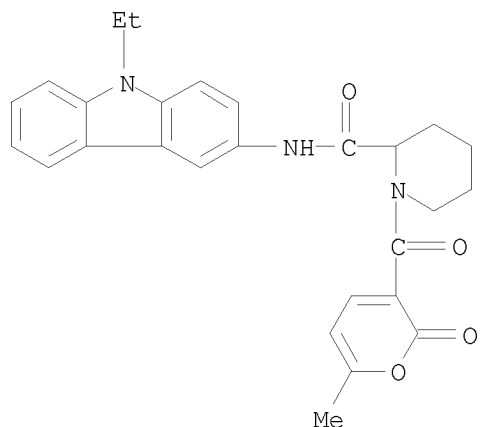


RN 258277-98-4 CAPLUS

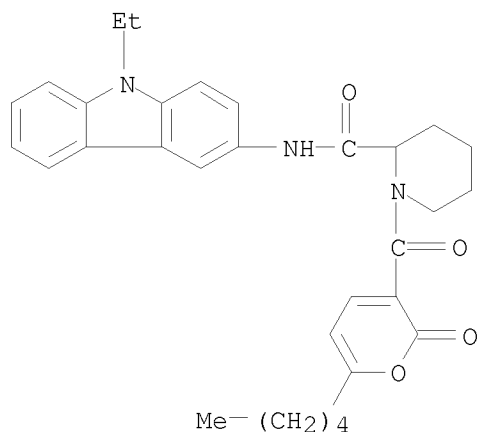
CN 2-Piperidinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1-[(2-oxo-6-phenyl-2H-pyran-3-yl)carbonyl]- (CA INDEX NAME)



RN 258277-99-5 CAPLUS
 CN 2-Piperidinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1-[(6-methyl-2-oxo-2H-pyran-3-yl)carbonyl]- (CA INDEX NAME)

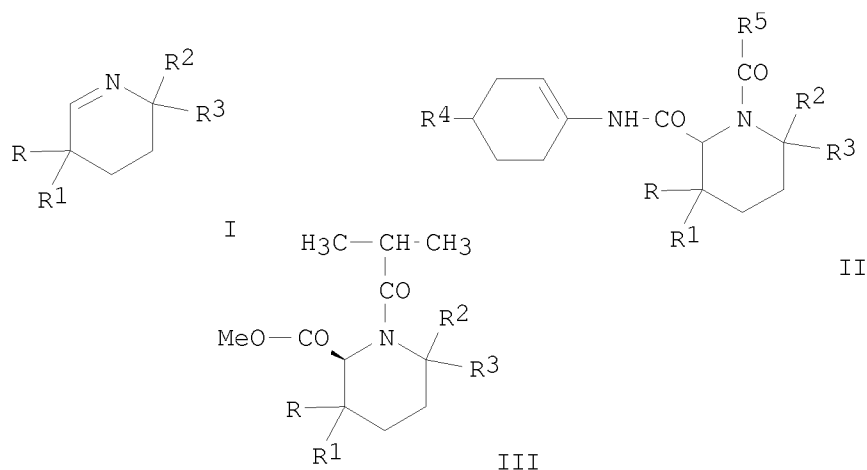


RN 258278-02-3 CAPLUS
 CN 2-Piperidinecarboxamide, N-(9-ethyl-9H-carbazol-3-yl)-1-[(2-oxo-6-pentyl-2H-pyran-3-yl)carbonyl]- (CA INDEX NAME)

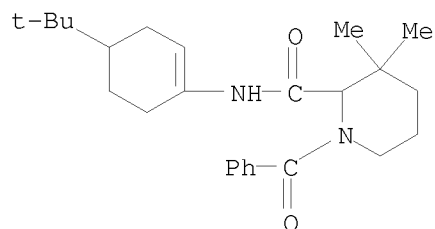


L4 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1999:758775 CAPLUS
 DOCUMENT NUMBER: 132:237328
 TITLE: Synthesis of novel pipecolic acid derivatives: a multicomponent approach from 3,4,5,6-tetrahydropyridines
 AUTHOR(S): Maison, Wolfgang; Lutzen, Arne; Kosten, Marc; Schlemminger, Imre; Westerhoff, Ole; Martens, Jurgen
 CORPORATE SOURCE: Department of Organic Chemistry, University of Oldenburg, Oldenburg, 26111, Germany
 SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1999), (23),
 3515-3525
 CODEN: JCPRB4; ISSN: 0300-922X
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 132:237328
 GI

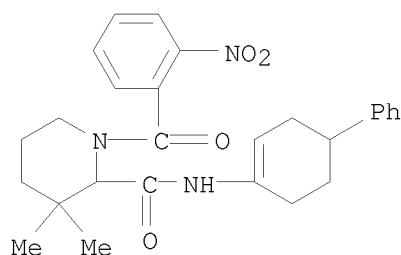


- AB A simple approach to several derivs. of pipecolic acid is via a multicomponent reaction starting from cyclic imines (I; R = Me, Et; R1 = Me, Et, Pr, Ph; R, R1 = (CH₂)₅; R2 = H, Me, Et, CH(CH₃)₂, Ph; R3 = H, Me, Ph), which are synthesized on a large scale and with different substitution patterns. The protected amino acids (II; R = Me, Et; R1 = Me, Et, Ph; R2 = H, Me, Ph; R3 = H, Me, Ph; R4 = H, C(CH₃)₃, Ph; R5 = Me, CH₂Cl, CH(CH₃)₂, Ph, 2-O₂N-C₆H₄-, 2,4-(MeO)-C₆H₃-) are formed in high yields. In cases where chiral imines are used the target compds. are obtained with remarkable diastereoselectivity. Bisamides II serve as versatile precursors for the preparation of a wide range of amino acid derivs. Different methods of hydrolysis of II lead to the free pipecolic acids or its derivs. Employment of methanol or ethanethiol as a nucleophile in the acid-mediated conversion of enamides II results in N-acylated amino acid esters (III; R = Me; R1 = Pr, Ph; R, R1 = (CH₂)₅; R2 = H, Me, Et, CH(CH₃)₂, Ph; R3 = H). Furthermore a method for the resolution of the obtained racemic α-amino acids via diastereomeric salt formation is described.
- IT 261917-72-0P 261917-74-2P 261917-75-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis of novel pipecolic acid derivs. from tetrahydropyridines via Ugi 3-component condensation)
- RN 261917-72-0 CAPLUS
- CN 2-Piperidinecarboxamide, 1-benzoyl-N-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl]-3,3-dimethyl- (CA INDEX NAME)



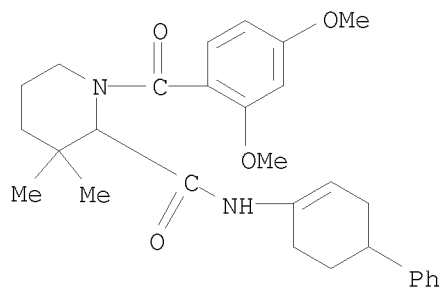
RN 261917-74-2 CAPLUS

CN 2-Piperidinecarboxamide, 3,3-dimethyl-1-(2-nitrobenzoyl)-N-(4-phenyl-1-cyclohexen-1-yl)- (CA INDEX NAME)



RN 261917-75-3 CAPLUS

CN 2-Piperidinecarboxamide, 1-(2,4-dimethoxybenzoyl)-3,3-dimethyl-N-(4-phenyl-1-cyclohexen-1-yl)- (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:709058 CAPLUS

DOCUMENT NUMBER: 129:343423

ORIGINAL REFERENCE NO.: 129:69949a,69952a

TITLE: 2-Benzoyl-1,2,3,4-tetrahydroisoquinoline-3-carboxamide derivatives and their use as inhibitors of hepatic production of ApoB-100

INVENTOR(S): Daugan, Alain Claude-Marie; Pianetti, Pascal Maurice Charles

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 60 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847877	A1	19981029	WO 1998-EP2244	19980420
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9875265	A	19981113	AU 1998-75265	19980420
IN 1998CA00672	A	20051202	IN 1998-CA672	19980420
PRIORITY APPLN. INFO.:			GB 1997-8119	A 19970422
			WO 1998-EP2244	W 19980420
OTHER SOURCE(S):	MARPAT 129:343423			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to compds. I [wherein R0 = H, halo, C1-4 alkyl, C1-4 alkoxy, or methylenedioxy; n = 1-4; R1 = H, halo, C1-4 alkyl, C1-4 alkoxy, CF3O, or methylenedioxy; p = 1-4; R2 = H, halo, C1-4 alkyl, C1-4 alkoxy, methylenedioxy, NR4R5, -(C1-4 alkylene)-NR6R7, -NR4- or -O-(C1-4 alkylene)-NR8R9, 4-morpholino, or 4-R10-piperazin-1-yl, m = 1-4; R3 = H or C1-4 alkyl; R4-R10 = H or C1-4 alkyl] and their pharmaceutically acceptable salts or solvates, to processes for their preparation, and their use in the treatment of conditions mediated by ApoB-100 regulation. In particular, as inhibitors of hepatic ApoB-100 production, I are of use in treatment of pancreatitis, NIDDM, coronary heart disease, hyperlipidemia, and hypercholesterolemia. For instance, (+)-7-methyl-1,2,3,4-tetrahydronaphthalen-1-ylamine (resolution given) was coupled with 2-BOC-D-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid using EDC and HOBT, and the resultant amide was deprotected with CF3CO2H and coupled with 4-MeC6H4CO2H under similar conditions to give title compound II (+)-isomer. In a test for potency and selectivity, II inhibited production of ApoB-100 in HepG2 cells in vitro with an IC50 of 0.9 nM, but showed an IC50 of > 5000 nM toward ApoA-1 production in the same assay. Almost 50 compds. were prepared, and their stereo-unspecified forms were claimed. Approx. 60 intermediates were prepared, 7 compds. were bioassayed, and 21 pharmaceutical formulations were listed.

IT 215314-12-8P 215314-13-9P 215314-14-0P
 215314-15-1P 215314-16-2P 215314-17-3P
 215314-18-4P 215314-19-5P 215314-20-8P
 215314-21-9P 215314-23-1P 215314-26-4P
 215314-27-5P 215314-29-7P 215314-31-1P
 215314-32-2P 215314-34-4P 215314-36-6P

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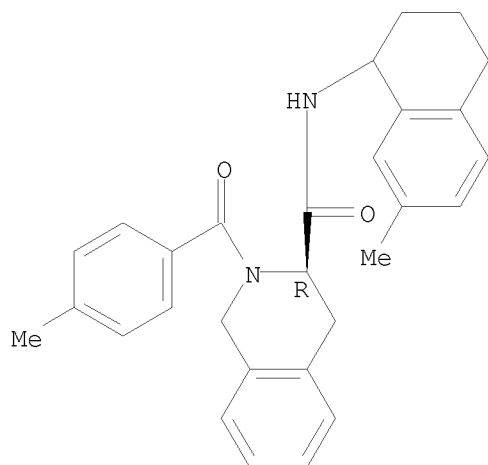
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(product; preparation of benzoyltetrahydroisoquinolinecarboxamide derivs. as inhibitors of hepatic production of ApoB-100)

RN 215314-12-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

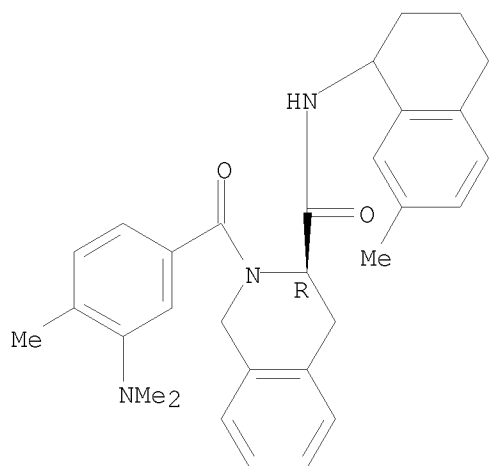
Absolute stereochemistry.



RN 215314-13-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)-4-methylbenzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

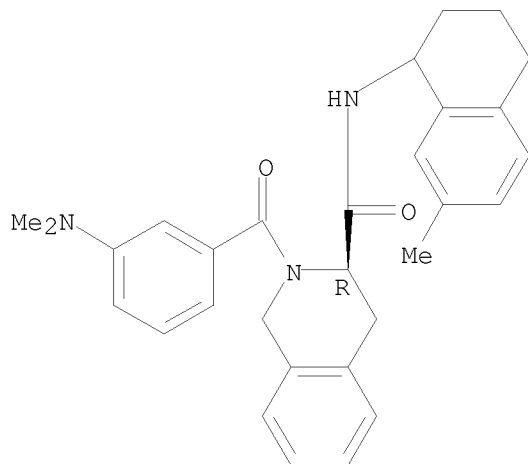
Absolute stereochemistry.



RN 215314-14-0 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

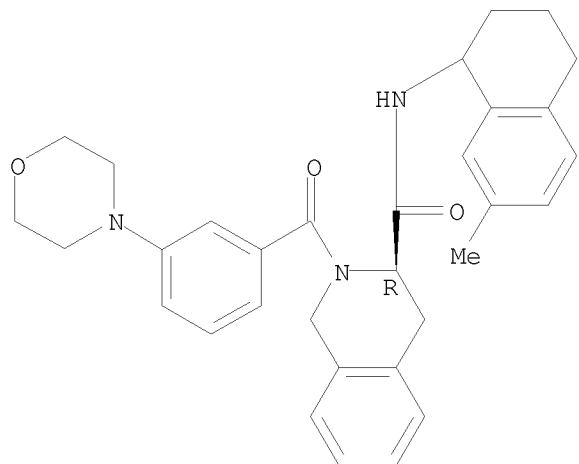
Absolute stereochemistry.



RN 215314-15-1 CAPLUS

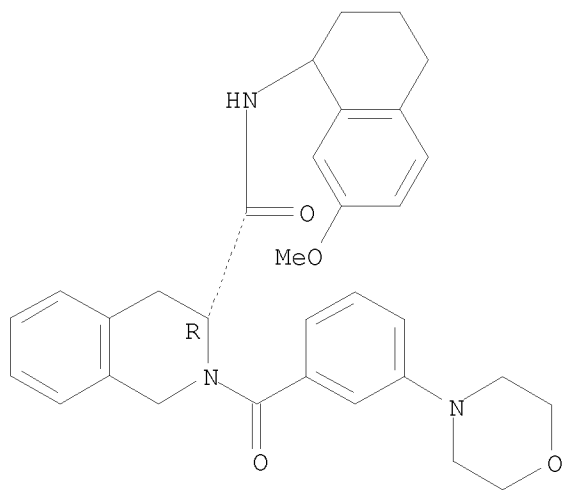
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



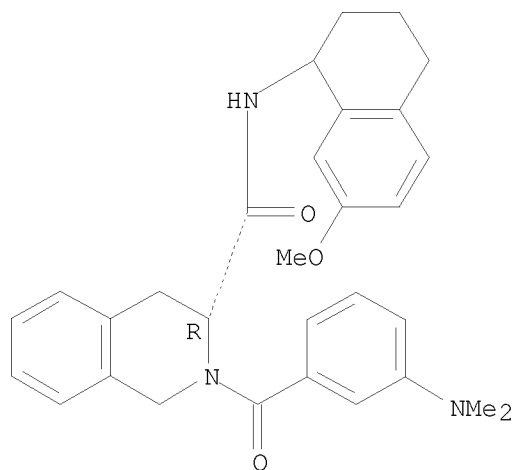
RN 215314-16-2 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 215314-17-3 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-
 N-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

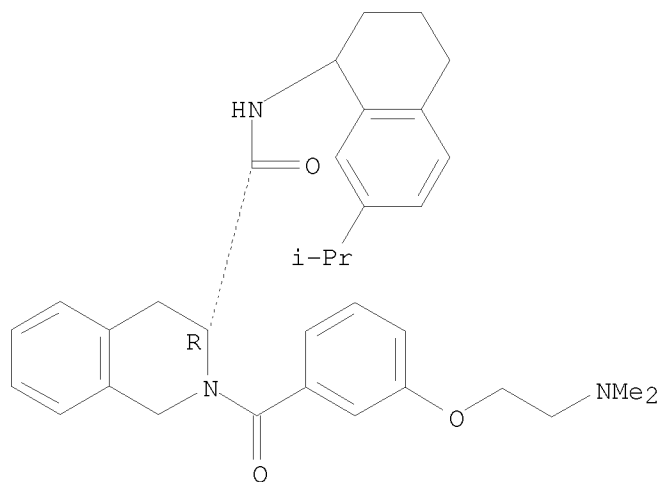
Absolute stereochemistry.



RN 215314-18-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, (3R)- (CA INDEX NAME)

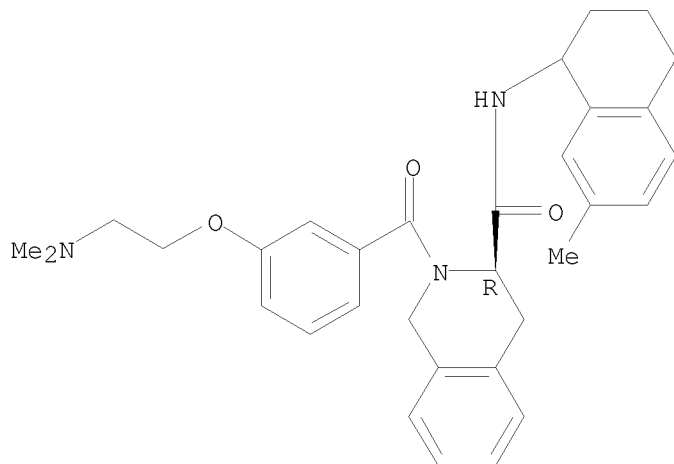
Absolute stereochemistry.



RN 215314-19-5 CAPLUS

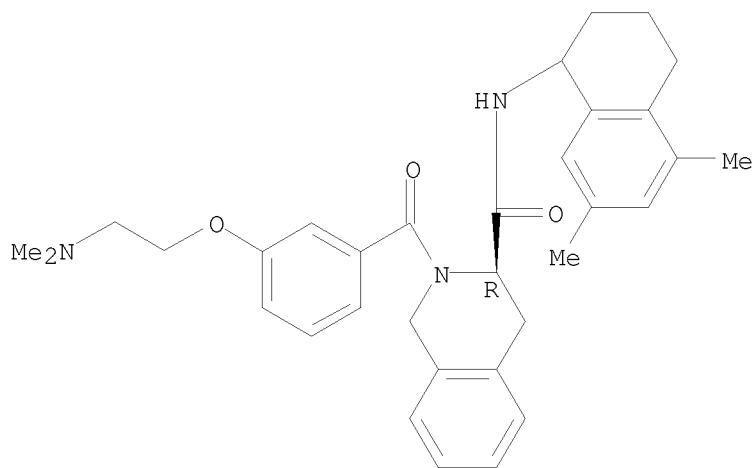
CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



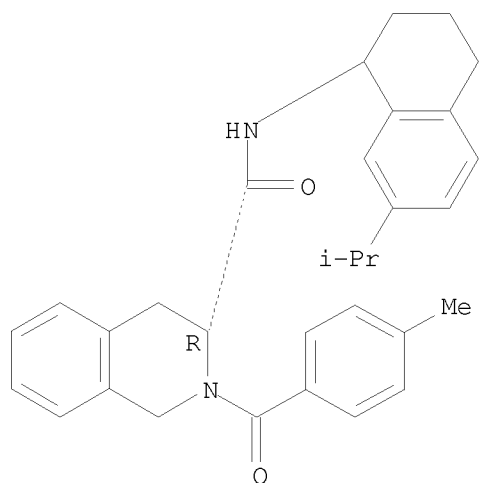
RN 215314-20-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



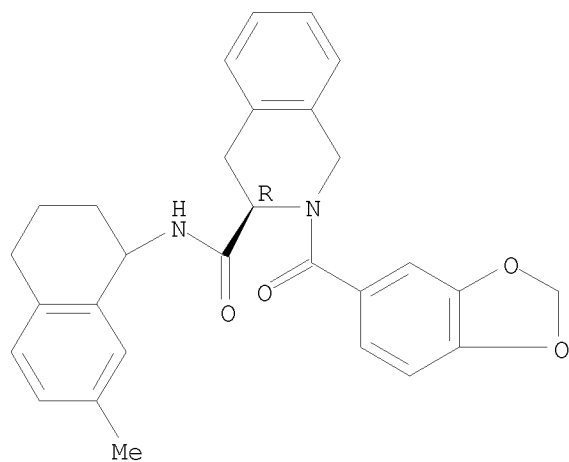
RN 215314-21-9 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



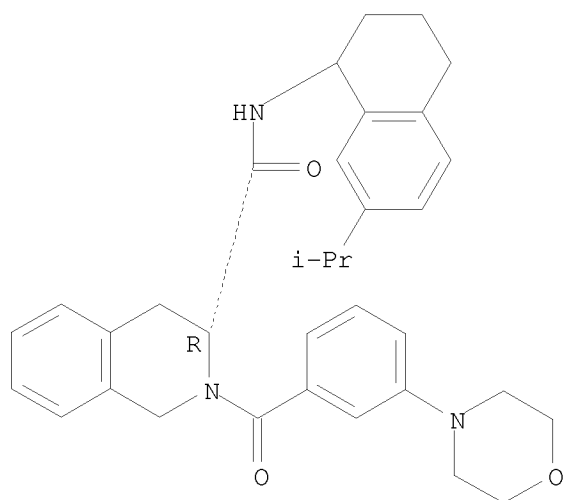
RN 215314-23-1 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-(1,3-benzodioxol-5-ylcarbonyl)-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 215314-26-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, (3R)- (CA INDEX NAME)

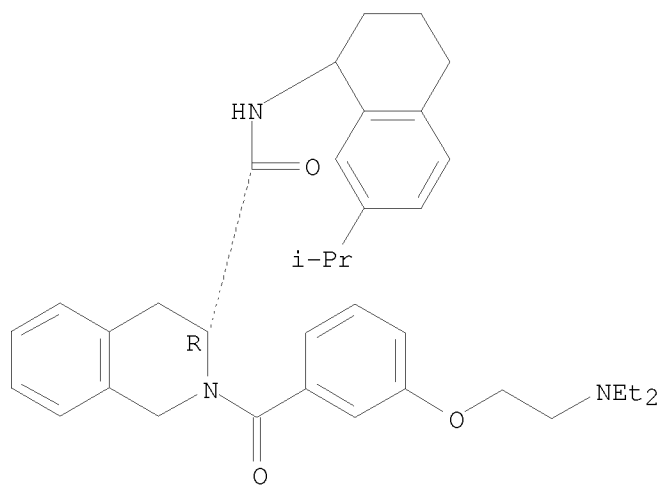
Absolute stereochemistry.



RN 215314-27-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(diethylamino)ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, (3R)- (CA INDEX NAME)

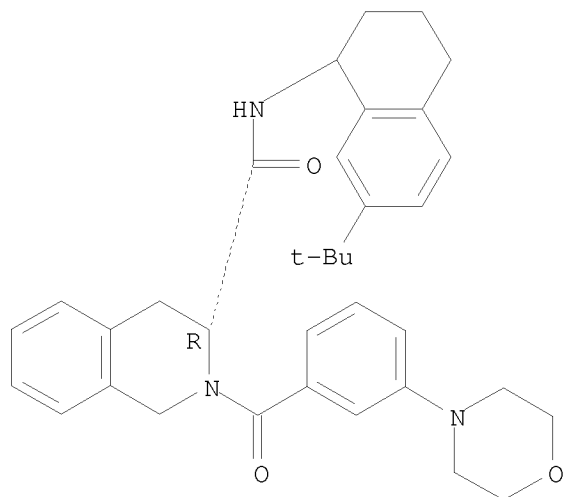
Absolute stereochemistry.



RN 215314-29-7 CAPLUS

CN 3-Isoquinolinecarboxamide, N-[7-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-1-naphthalenyl]-1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-, (3R)- (CA INDEX NAME)

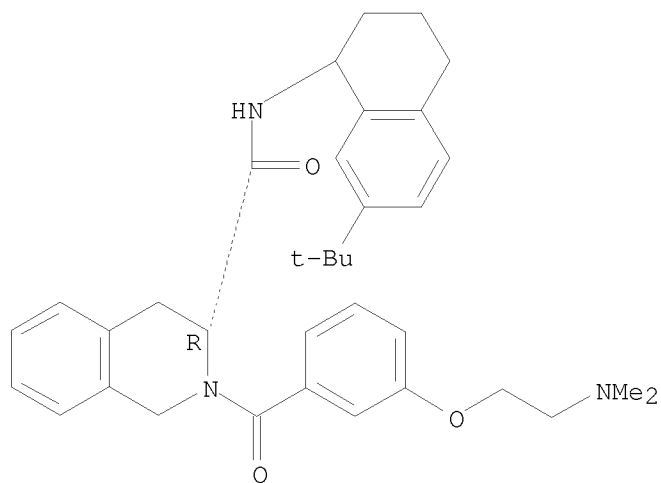
Absolute stereochemistry.



RN 215314-31-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-N-[7-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-1-naphthalenyl]-1,2,3,4-tetrahydro-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

Absolute stereochemistry.

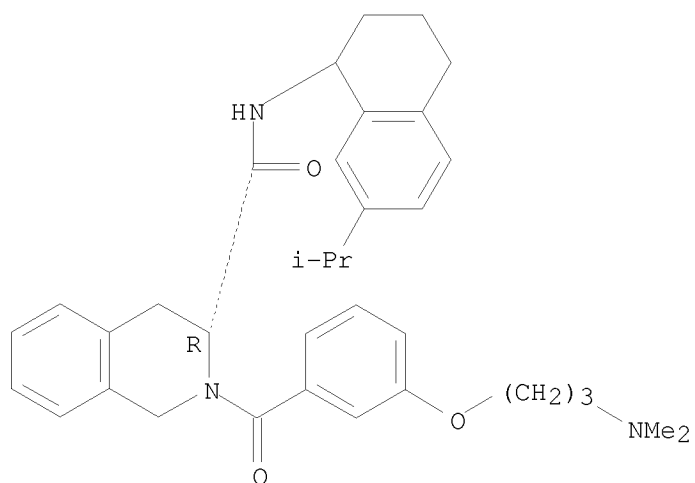


● HCl

RN 215314-32-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[3-(dimethylamino)propoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

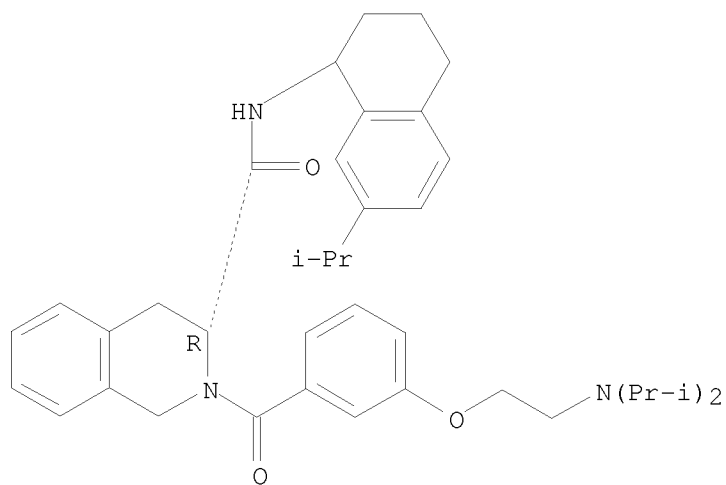
Absolute stereochemistry.



● HCl

RN 215314-34-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-[2-[bis(1-methylethyl)amino]ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

Absolute stereochemistry.

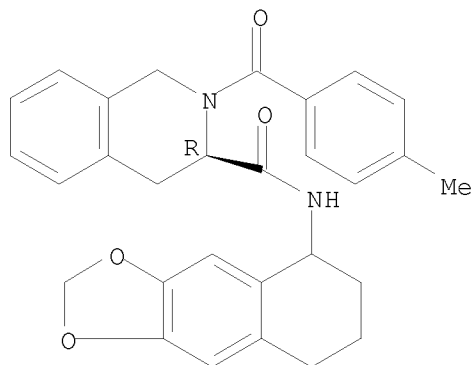


● HCl

RN 215314-36-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-(5,6,7,8-tetrahydronaphtho[2,3-d]-1,3-dioxol-5-yl)-, (3R)- (CA INDEX NAME)

NAME)

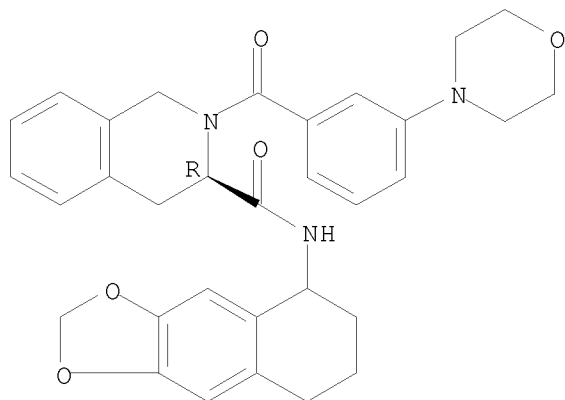
Absolute stereochemistry.



RN 215314-38-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-N-(5,6,7,8-tetrahydronaphtho[2,3-d]-1,3-dioxol-5-yl)-, (3R)- (CA INDEX NAME)

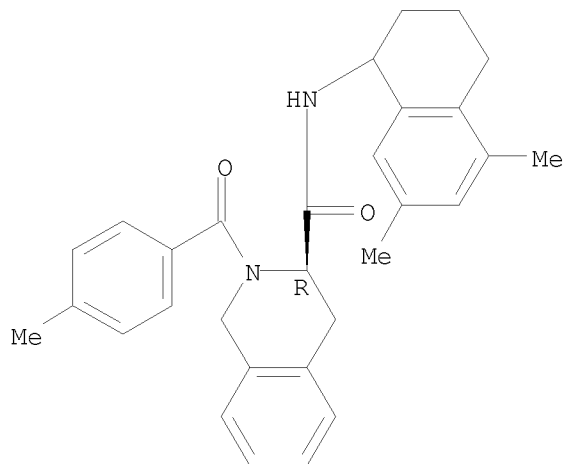
Absolute stereochemistry.



RN 215314-40-2 CAPLUS

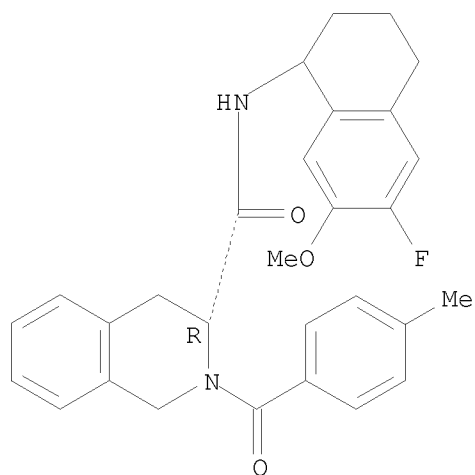
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-(1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



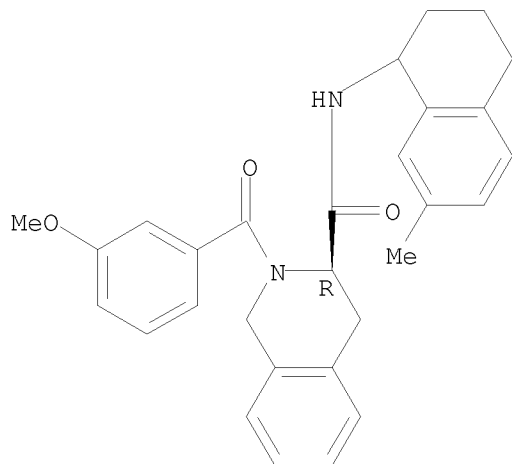
RN 215314-42-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-(6-fluoro-1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)-1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



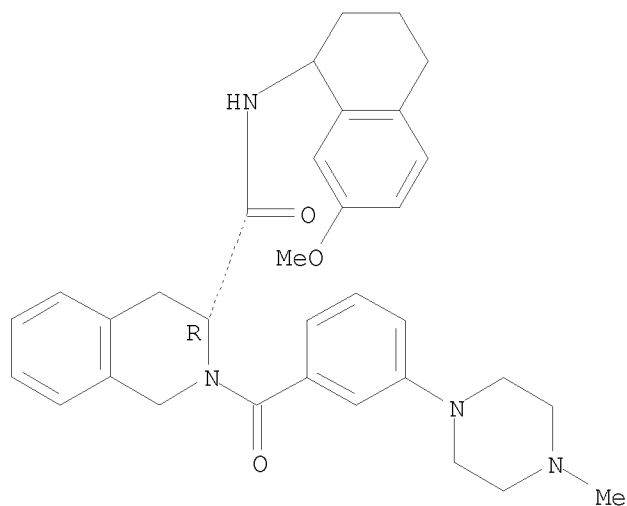
RN 215314-45-7 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-methoxybenzoyl)-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



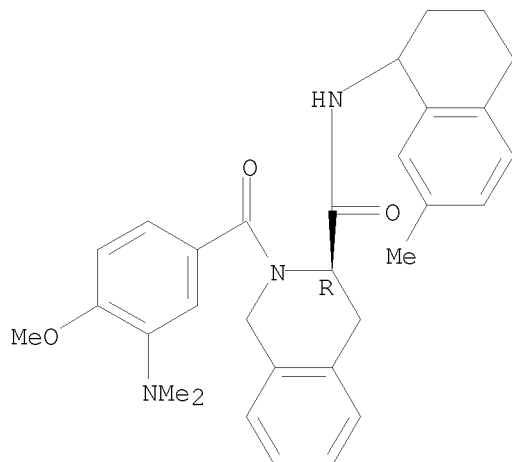
RN 215314-46-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-methyl-1-piperazinyl)benzoyl]-N-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 215314-48-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)-4-methoxybenzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

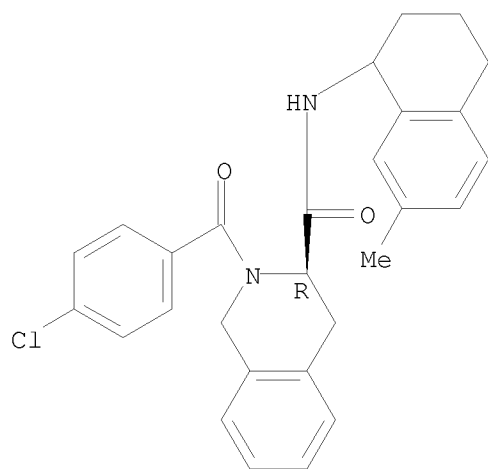
Absolute stereochemistry.



RN 215314-50-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(4-chlorobenzoyl)-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

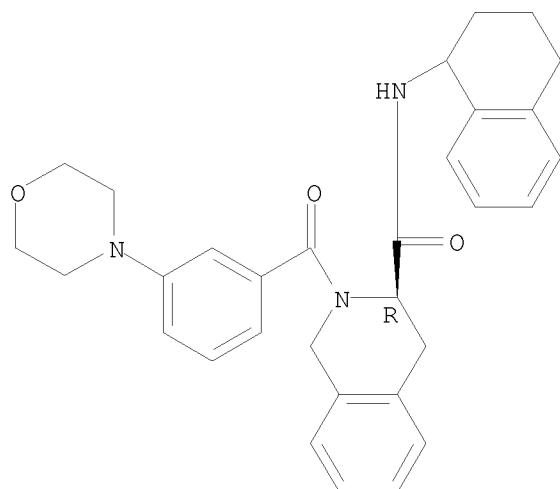
Absolute stereochemistry.



RN 215314-52-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-N-(1,2,3,4-tetrahydro-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

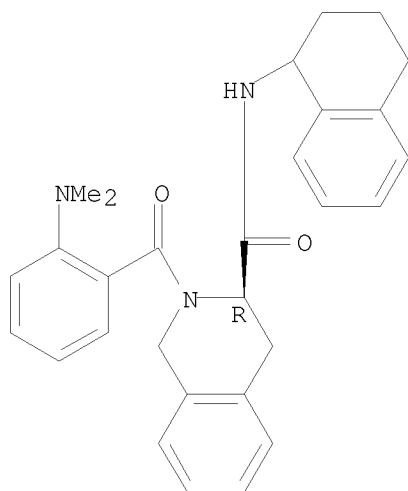
Absolute stereochemistry.



RN 215314-54-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[2-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-1-naphthalenyl)-, (3R)- (CA INDEX NAME)

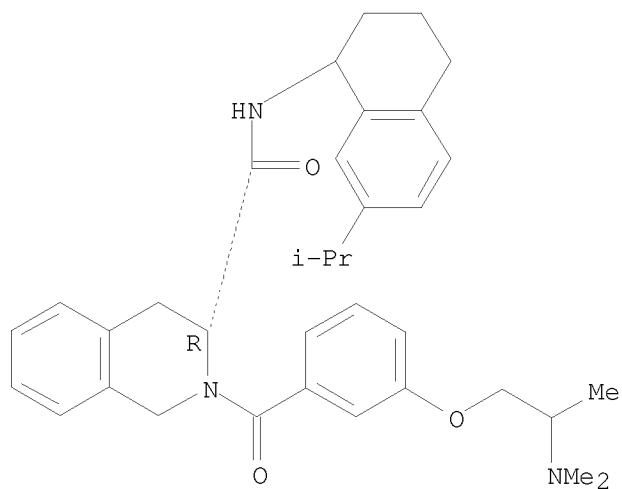
Absolute stereochemistry.



RN 215314-55-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)propoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

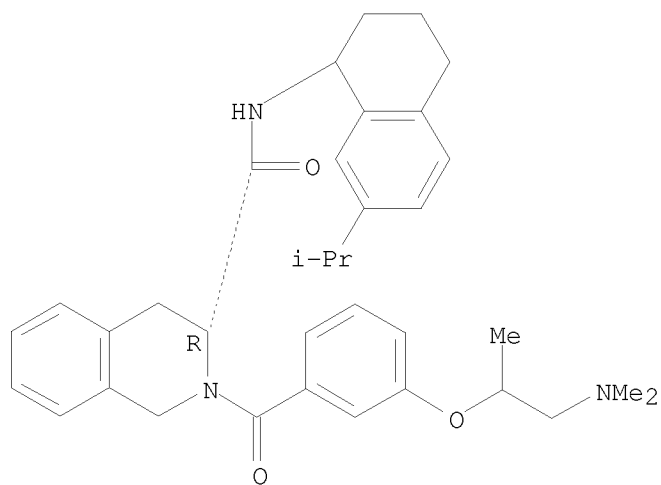
Absolute stereochemistry.



● HCl

RN 215314-56-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)-1-methylethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

Absolute stereochemistry.

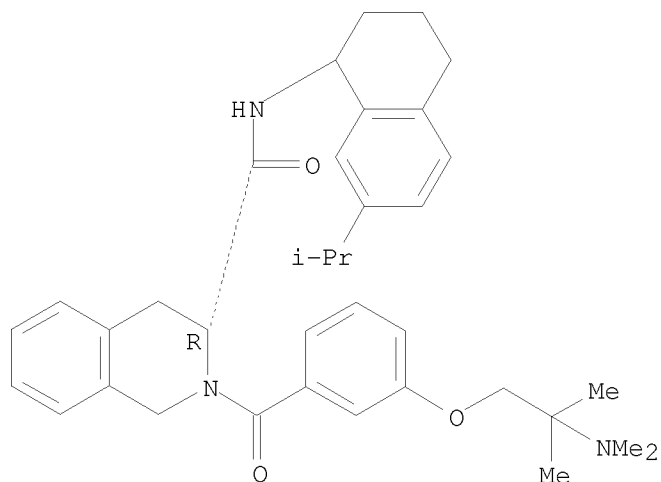


● HCl

RN 215314-58-2 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)-2-methylpropoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

methylethyl)-1-naphthalenyl]-, (3R)- (CA INDEX NAME)

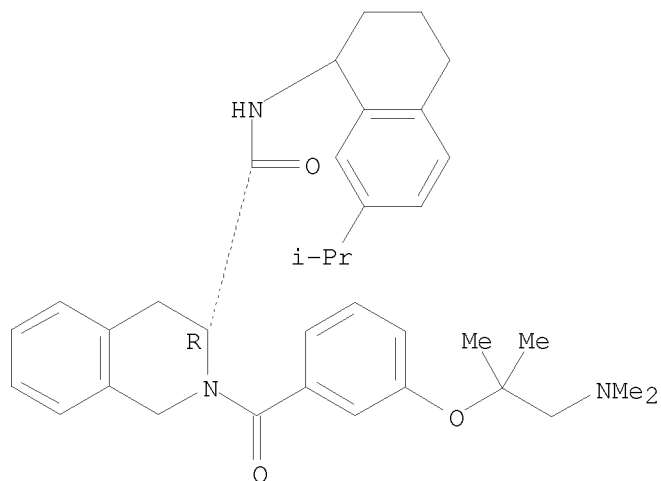
Absolute stereochemistry.



RN 215314-60-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)-1,1-dimethylethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

Absolute stereochemistry.

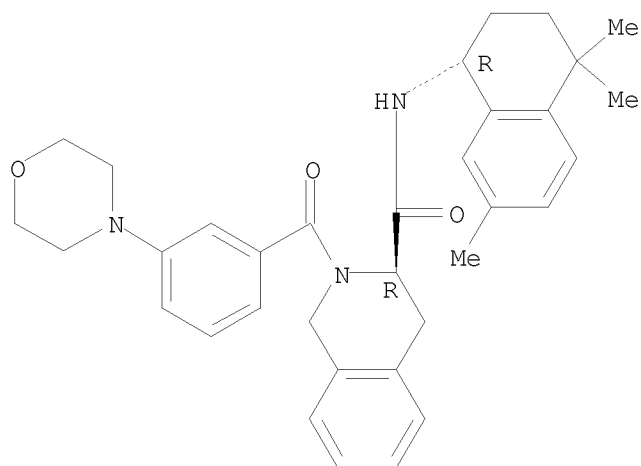


● HCl

RN 215314-62-8 CAPLUS

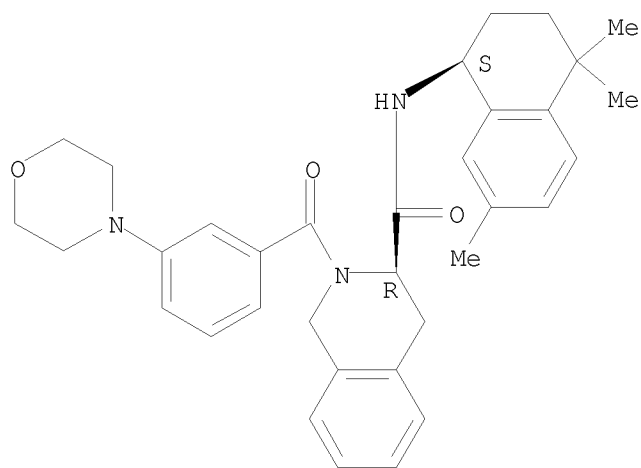
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-N-[(1R)-1,2,3,4-tetrahydro-4,4,7-trimethyl-1-naphthalenyl]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



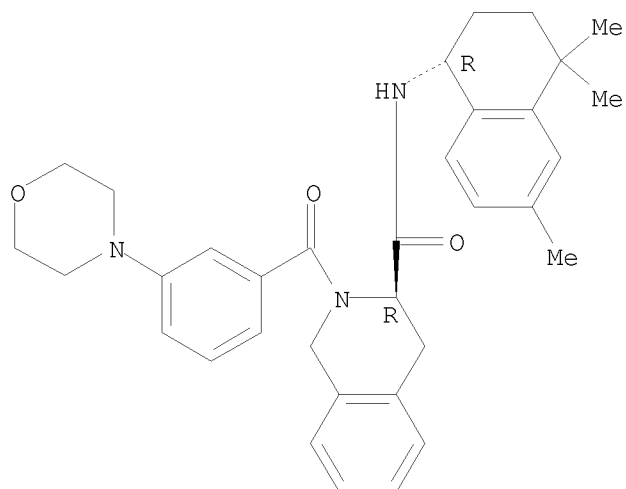
RN 215314-64-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1S)-1,2,3,4-tetrahydro-4,4,7-trimethyl-1-naphthalenyl]-, (3R)- (CA
 INDEX NAME)

Absolute stereochemistry. Rotation (+).



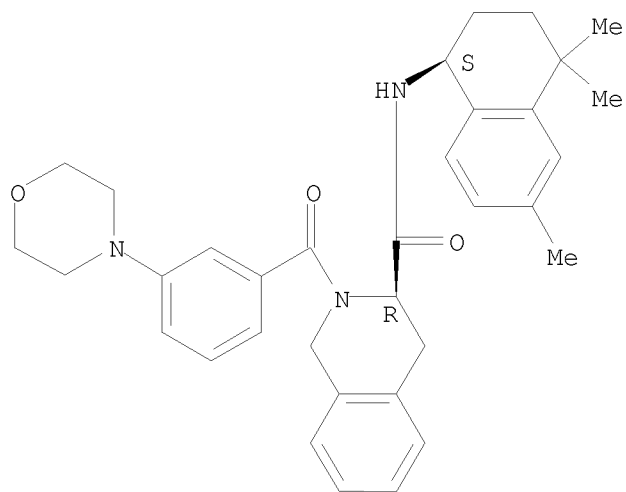
RN 215314-66-2 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-4,4,6-trimethyl-1-naphthalenyl]-, (3R)- (CA
 INDEX NAME)

Absolute stereochemistry. Rotation (+).



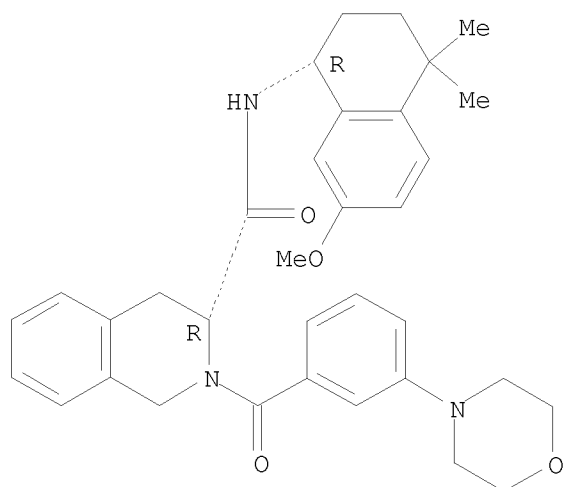
RN 215314-68-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1S)-1,2,3,4-tetrahydro-4,4,6-trimethyl-1-naphthalenyl]-, (3R)- (CA
 INDEX NAME)

Absolute stereochemistry. Rotation (+).



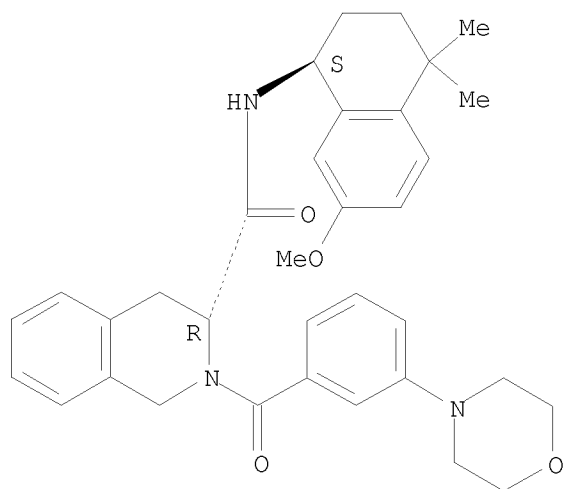
RN 215314-70-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-7-methoxy-4,4-dimethyl-1-naphthalenyl]-, (3R)-
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



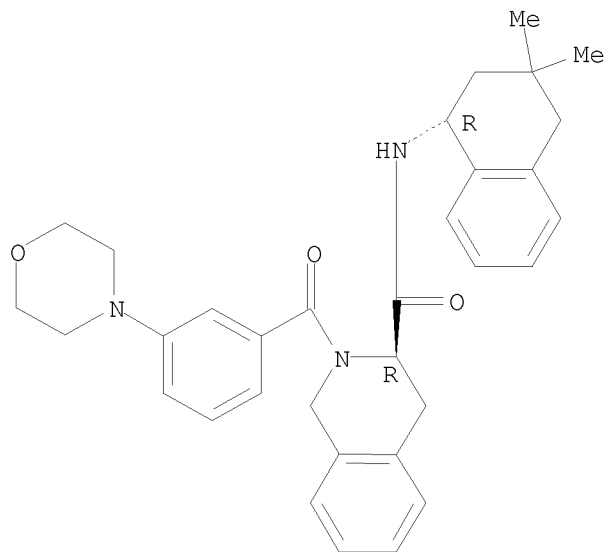
RN 215314-72-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1S)-1,2,3,4-tetrahydro-7-methoxy-4,4-dimethyl-1-naphthalenyl]-, (3R)-
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



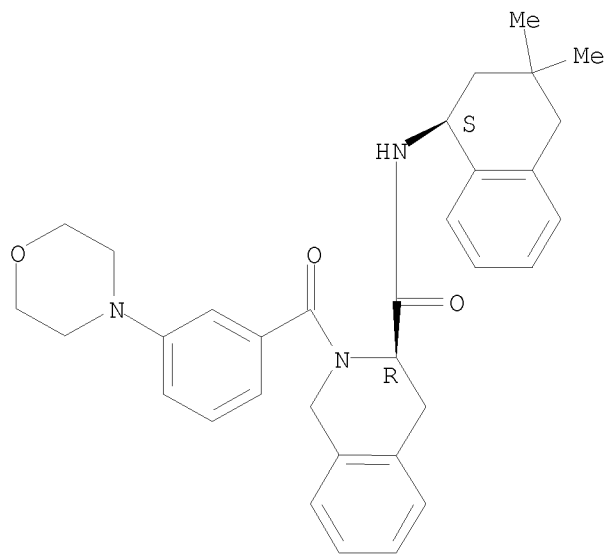
RN 215314-73-1 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-3,3-dimethyl-1-naphthalenyl]-, (3R)- (CA INDEX
 NAME)

Absolute stereochemistry. Rotation (+).



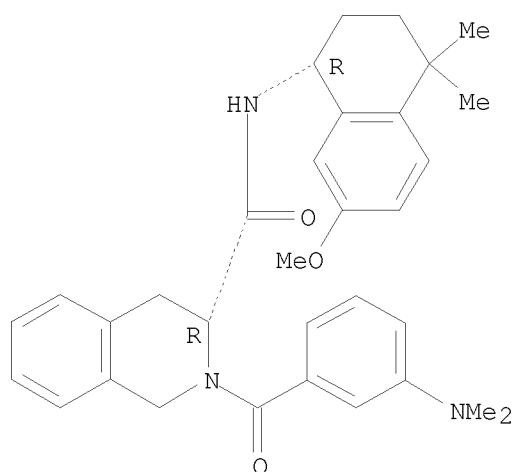
RN 215314-75-3 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1S)-1,2,3,4-tetrahydro-3,3-dimethyl-1-naphthalenyl]-, (3R)- (CA INDEX
 NAME)

Absolute stereochemistry. Rotation (+).



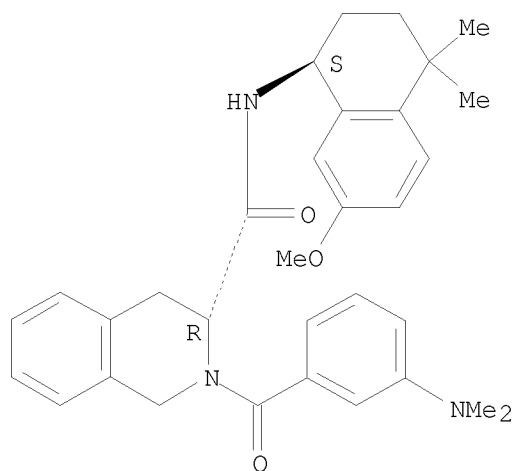
RN 215314-77-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-
 N-[(1R)-1,2,3,4-tetrahydro-7-methoxy-4,4-dimethyl-1-naphthalenyl]-, (3R)-
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



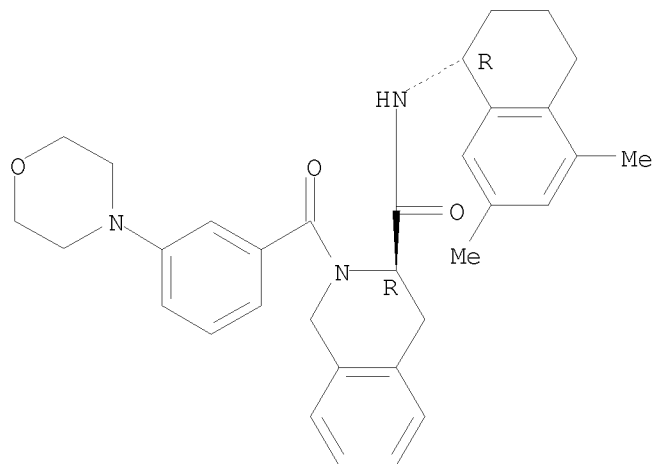
RN 215314-79-7 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-
 N-[(1S)-1,2,3,4-tetrahydro-7-methoxy-4,4-dimethyl-1-naphthalenyl]-, (3R)-
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



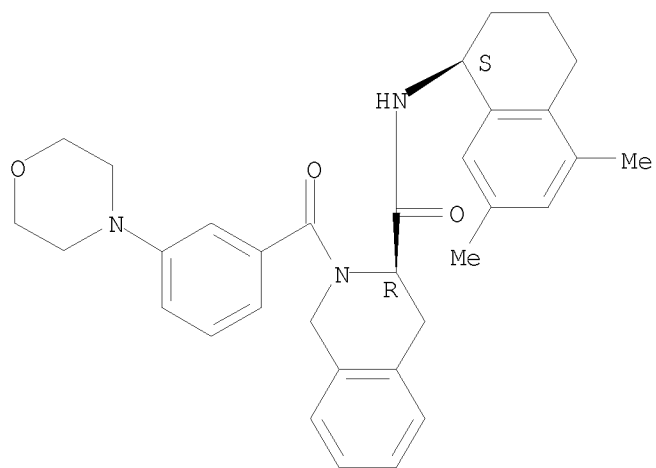
RN 215314-82-2 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl]-, (3R)- (CA INDEX
 NAME)

Absolute stereochemistry. Rotation (+).



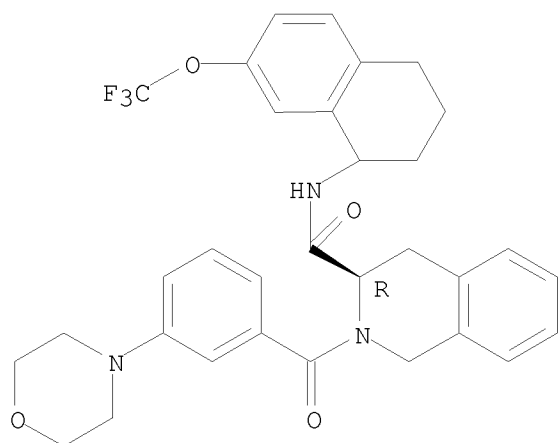
RN 215314-84-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1S)-1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl]-, (3R)- (CA INDEX
 NAME)

Absolute stereochemistry. Rotation (+).



RN 215314-87-7 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[1,2,3,4-tetrahydro-7-(trifluoromethoxy)-1-naphthalenyl]-, (3R)- (CA
 INDEX NAME)

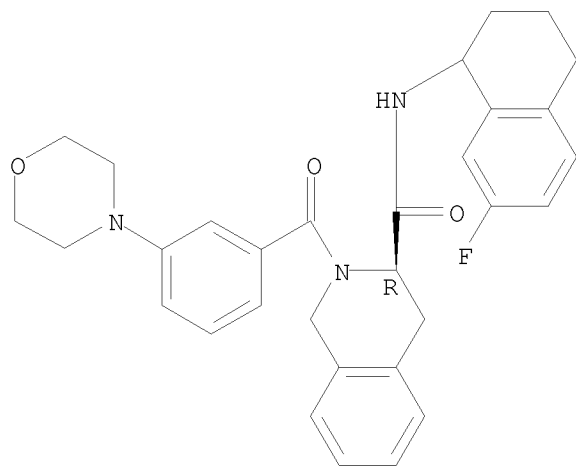
Absolute stereochemistry.



RN 215314-89-9 CAPLUS

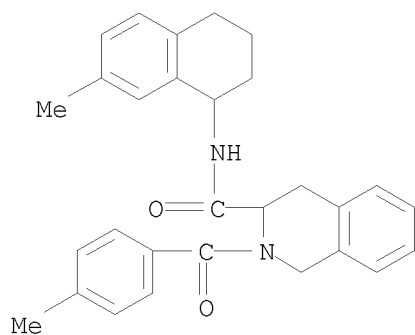
CN 3-Isoquinolinecarboxamide, N-(7-fluoro-1,2,3,4-tetrahydro-1-naphthalenyl)-1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



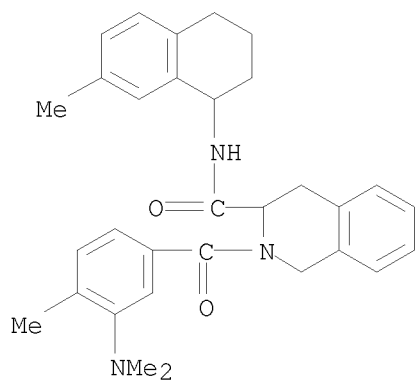
RN 215314-91-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



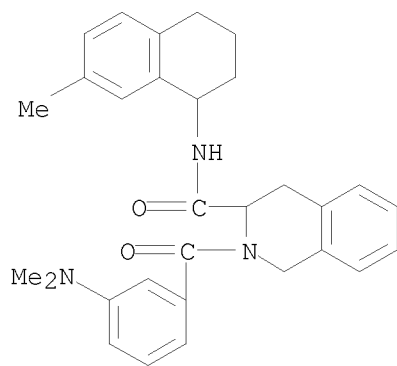
RN 215314-93-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)-4-methylbenzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



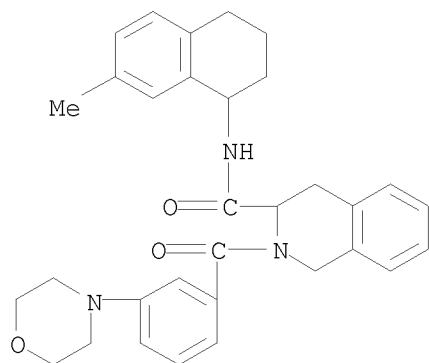
RN 215314-95-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



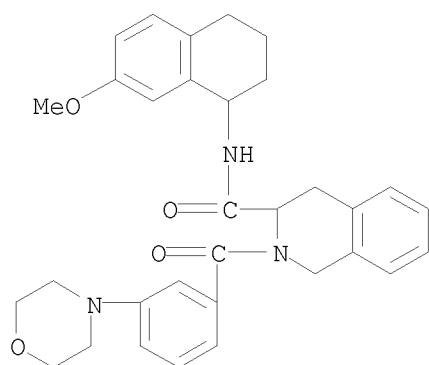
RN 215314-97-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



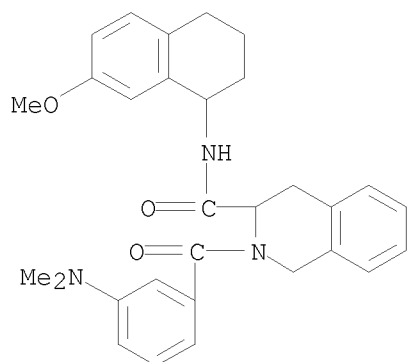
RN 215314-99-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
N-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)- (CA INDEX NAME)



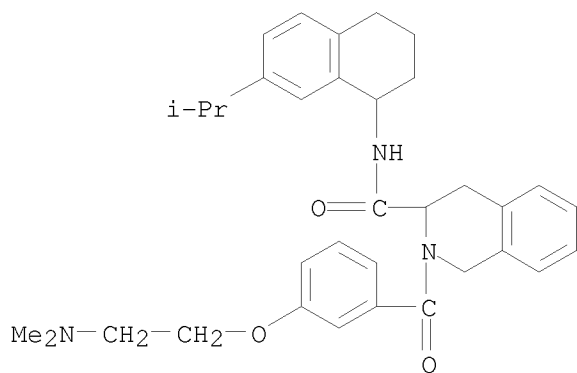
RN 215315-01-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-
N-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)- (CA INDEX NAME)



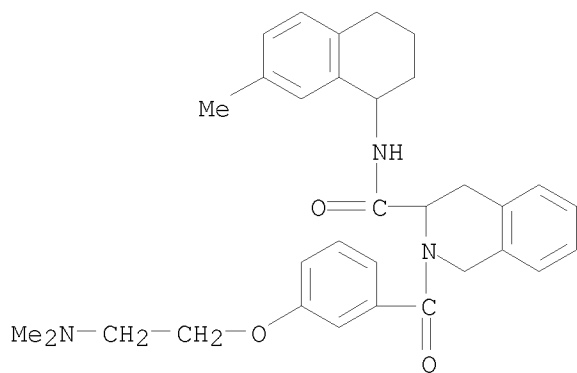
RN 215315-02-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]- (CA INDEX NAME)



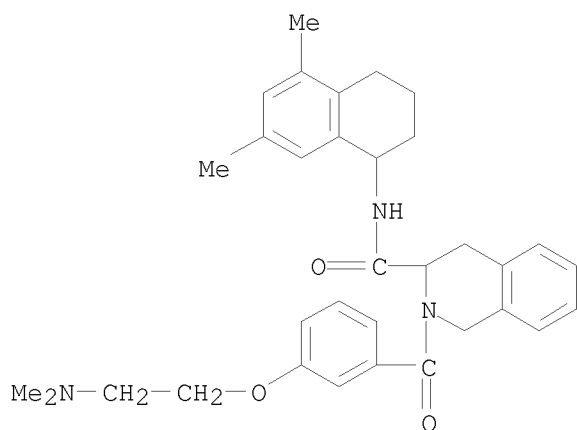
RN 215315-04-1 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



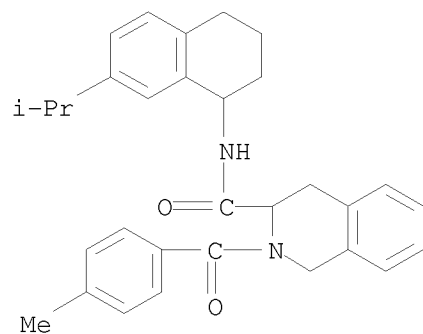
RN 215315-05-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl)- (CA INDEX NAME)



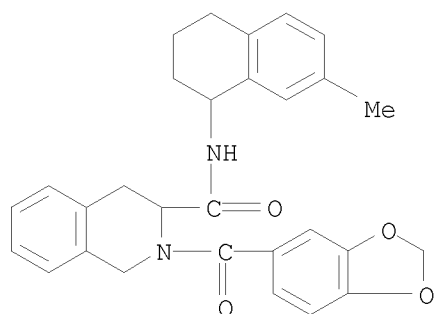
RN 215315-06-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]- (CA INDEX NAME)

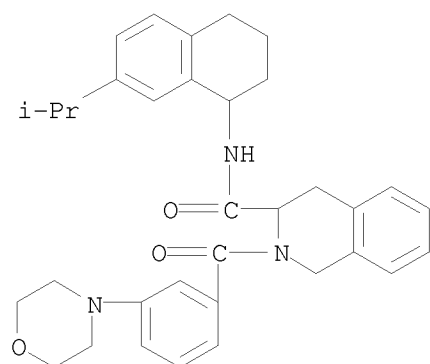


RN 215315-07-4 CAPLUS

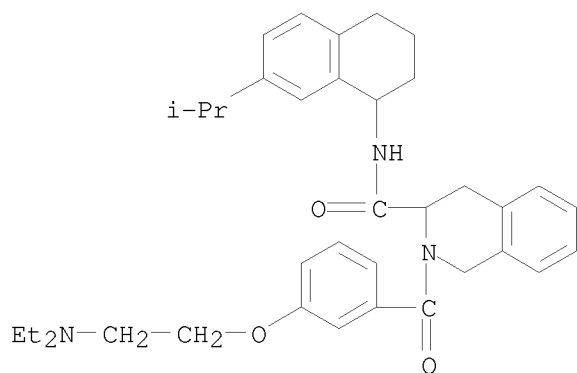
CN 3-Isoquinolinecarboxamide, 2-(1,3-benzodioxol-5-ylcarbonyl)-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



RN 215315-08-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]- (CA INDEX NAME)

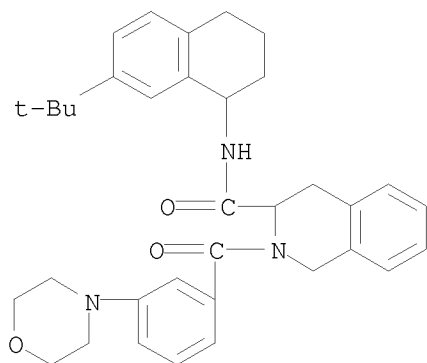


RN 215315-09-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-[2-(diethylamino)ethoxy]benzoyl]-1,2,3,4-
 tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]- (CA
 INDEX NAME)



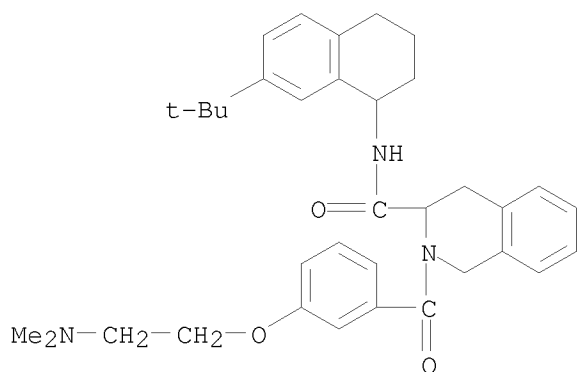
RN 215315-11-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, N-[7-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-1-

naphthalenyl]-1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]- (CA INDEX NAME)



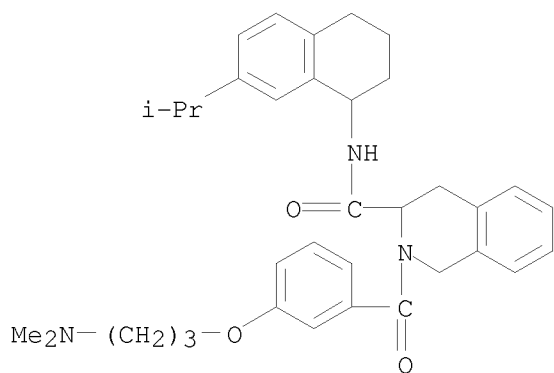
RN 215315-13-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)ethoxy]benzoyl]-N-[7-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-1-naphthalenyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)

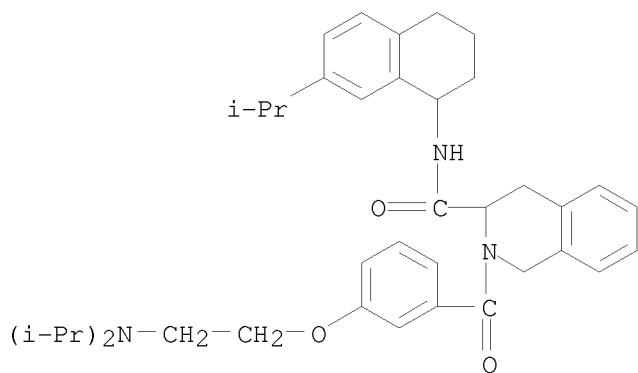


RN 215315-15-4 CAPLUS

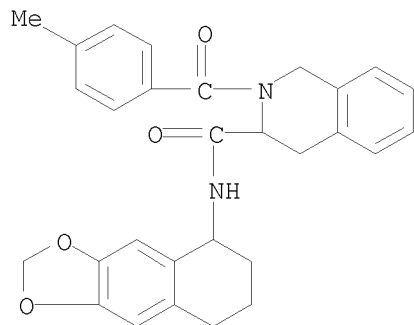
CN 3-Isoquinolinecarboxamide, 2-[3-[3-(dimethylamino)propoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]- (CA INDEX NAME)



RN 215315-16-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-[2-[bis(1-methylethyl)amino]ethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]- (CA INDEX NAME)

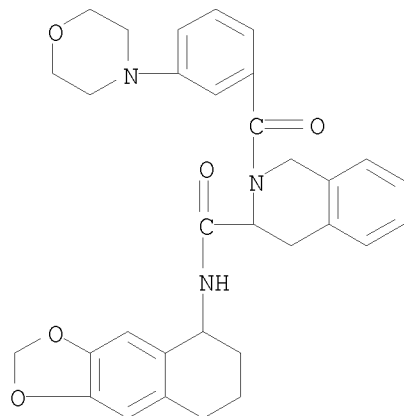


RN 215315-17-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-(5,6,7,8-tetrahydronaphtho[2,3-d]-1,3-dioxol-5-yl)- (CA INDEX NAME)



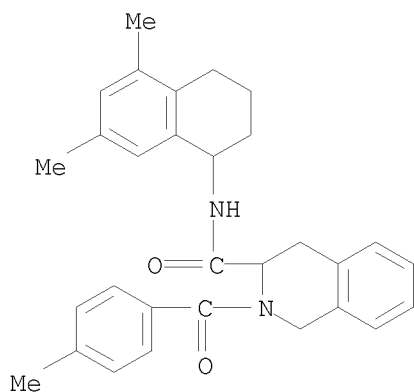
RN 215315-18-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
N-(5,6,7,8-tetrahydronaphtho[2,3-d]-1,3-dioxol-5-yl)- (CA INDEX NAME)



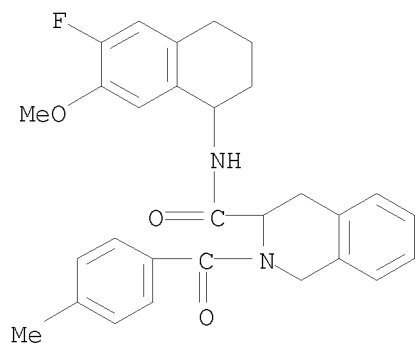
RN 215315-19-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(4-methylbenzoyl)-N-(1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl)- (CA INDEX NAME)



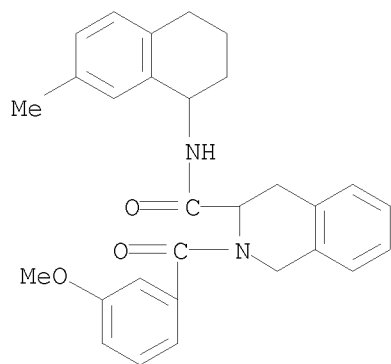
RN 215315-20-1 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(6-fluoro-1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)-1,2,3,4-tetrahydro-2-(4-methylbenzoyl)- (CA INDEX NAME)



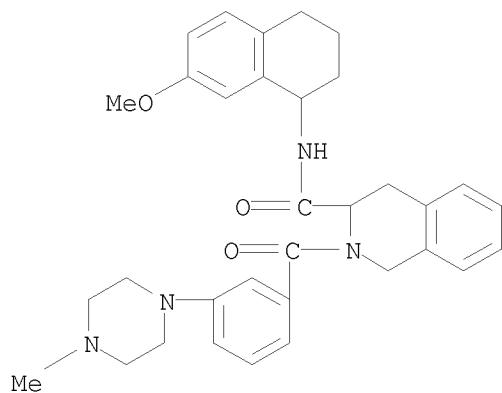
RN 215315-21-2 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-(3-methoxybenzoyl)-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



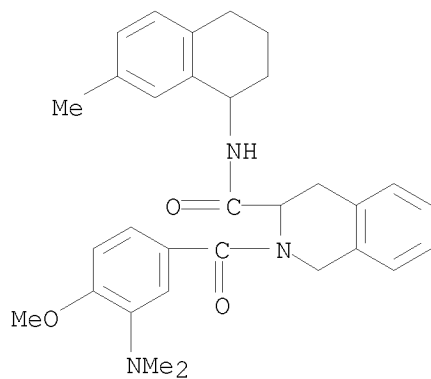
RN 215315-22-3 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-methyl-1-piperazinyl)benzoyl]-N-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)- (CA INDEX NAME)



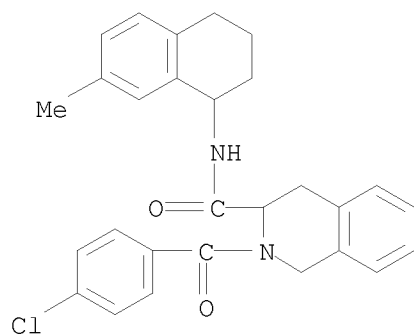
RN 215315-23-4 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)-4-methoxybenzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



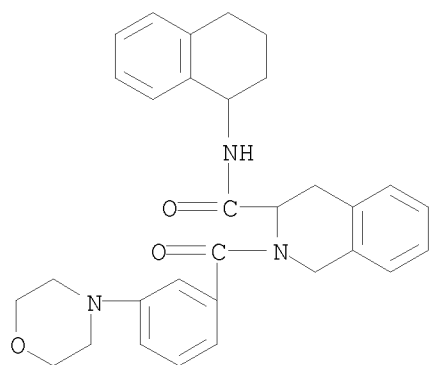
RN 215315-24-5 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-(4-chlorobenzoyl)-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-7-methyl-1-naphthalenyl)- (CA INDEX NAME)



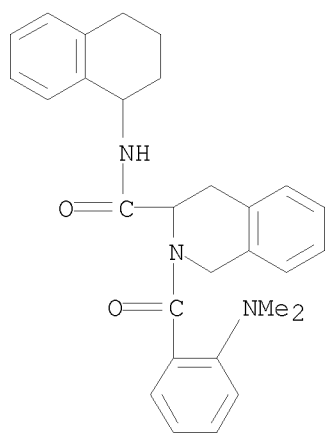
RN 215315-25-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-N-(1,2,3,4-tetrahydro-1-naphthalenyl)- (CA INDEX NAME)



RN 215315-26-7 CAPLUS

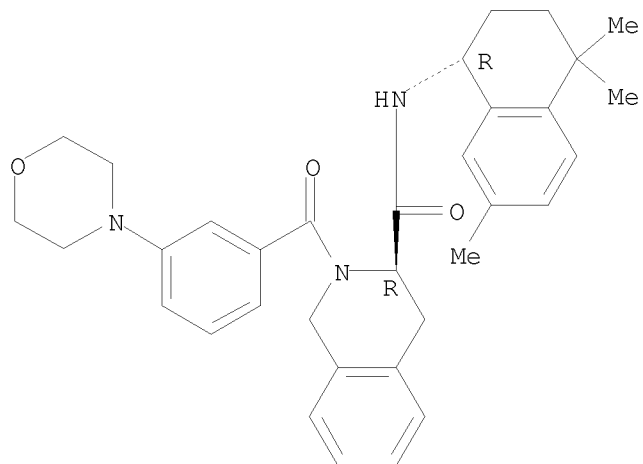
CN 3-Isoquinolinecarboxamide, 2-[2-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-N-(1,2,3,4-tetrahydro-1-naphthalenyl)- (CA INDEX NAME)



RN 215315-27-8 CAPLUS

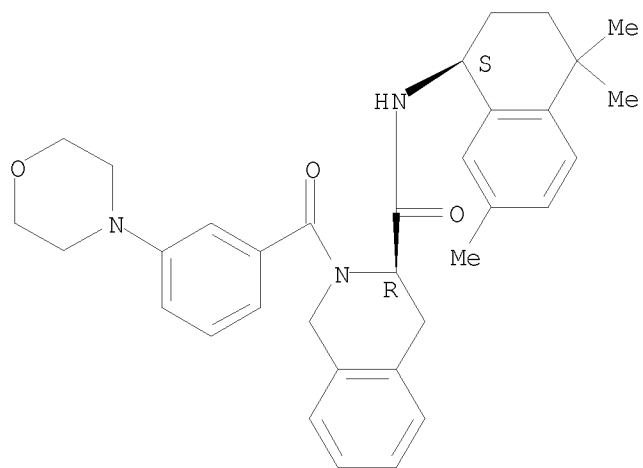
CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-N-[(1R)-1,2,3,4-tetrahydro-4,4,7-trimethyl-1-naphthalenyl]-, (3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



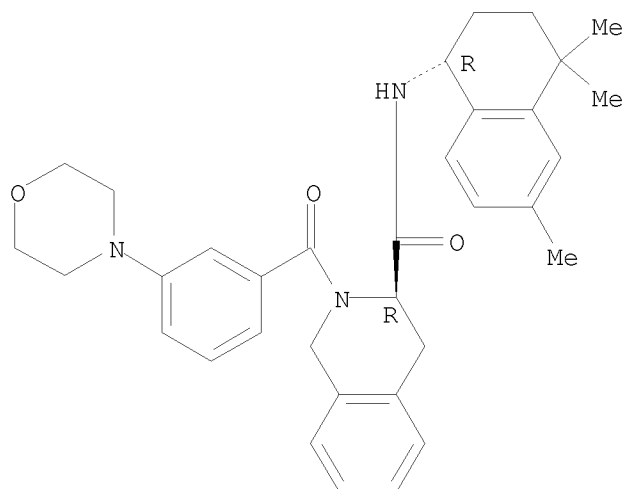
RN 215315-28-9 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-4,4,7-trimethyl-1-naphthalenyl]-, (3S)-rel-
 (CA INDEX NAME)

Relative stereochemistry.



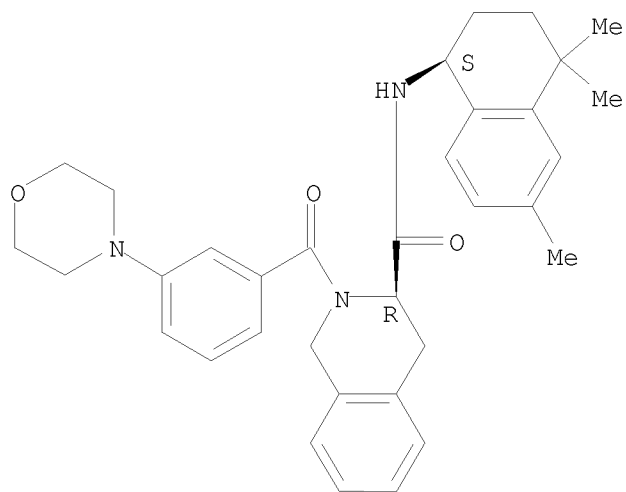
RN 215315-29-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-4,4,6-trimethyl-1-naphthalenyl]-, (3R)-rel-
 (CA INDEX NAME)

Relative stereochemistry.



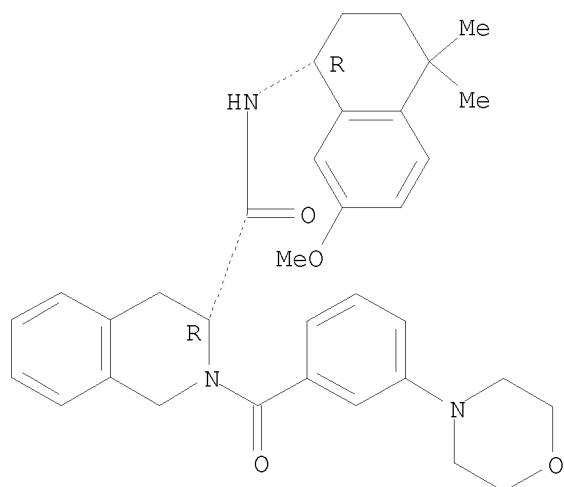
RN 215315-30-3 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-4,4,6-trimethyl-1-naphthalenyl]-, (3S)-rel-
 (CA INDEX NAME)

Relative stereochemistry.



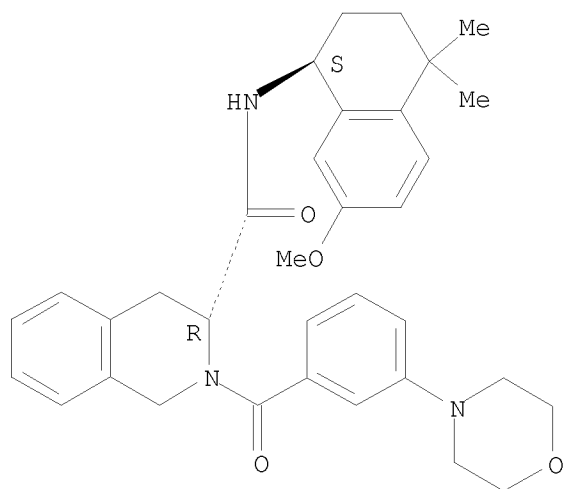
RN 215315-31-4 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-7-methoxy-4,4-dimethyl-1-naphthalenyl]-,
 (3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



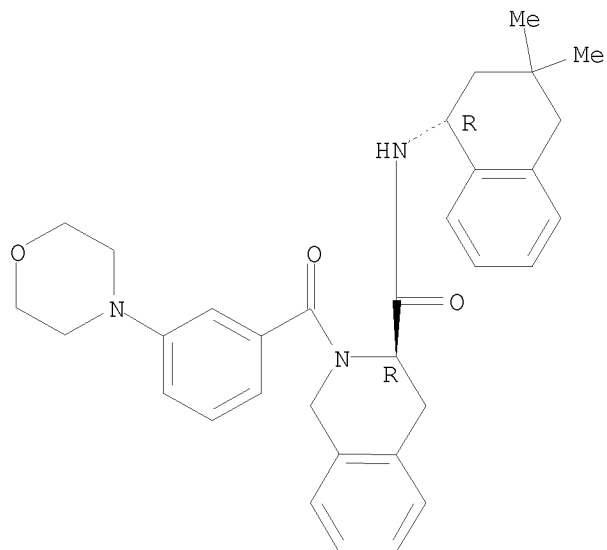
RN 215315-32-5 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-7-methoxy-4,4-dimethyl-1-naphthalenyl]-,
 (3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



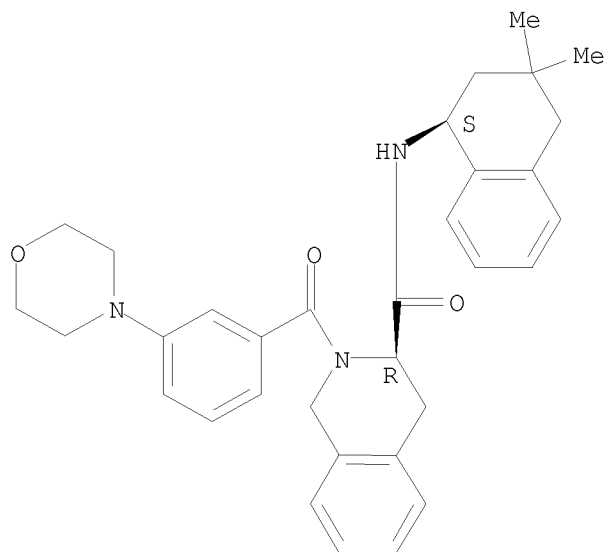
RN 215315-33-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-3,3-dimethyl-1-naphthalenyl]-, (3R)-rel- (CA
 INDEX NAME)

Relative stereochemistry.



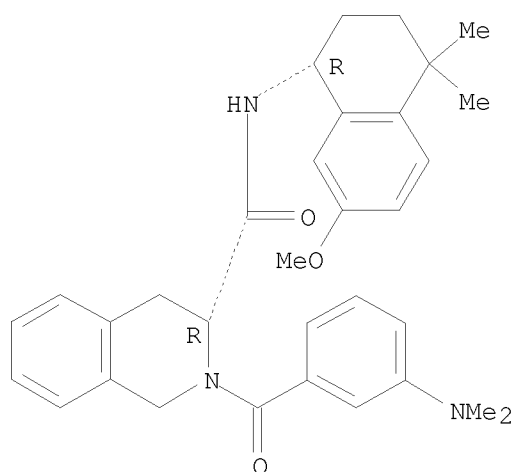
RN 215315-34-7 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-3,3-dimethyl-1-naphthalenyl]-, (3S)-rel- (CA
 INDEX NAME)

Relative stereochemistry.



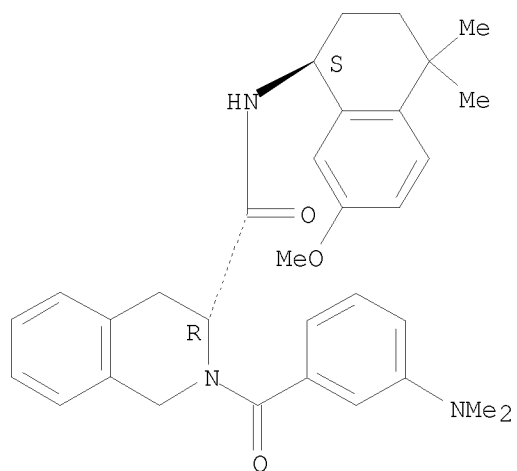
RN 215315-35-8 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-
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 (3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



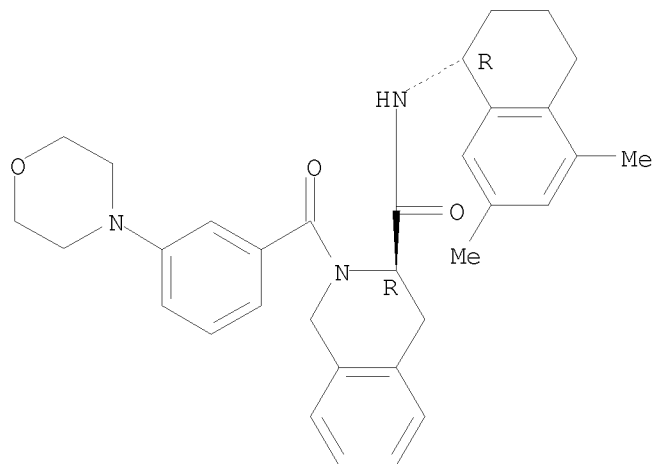
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 CN 3-Isoquinolinecarboxamide, 2-[3-(dimethylamino)benzoyl]-1,2,3,4-tetrahydro-
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 (3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



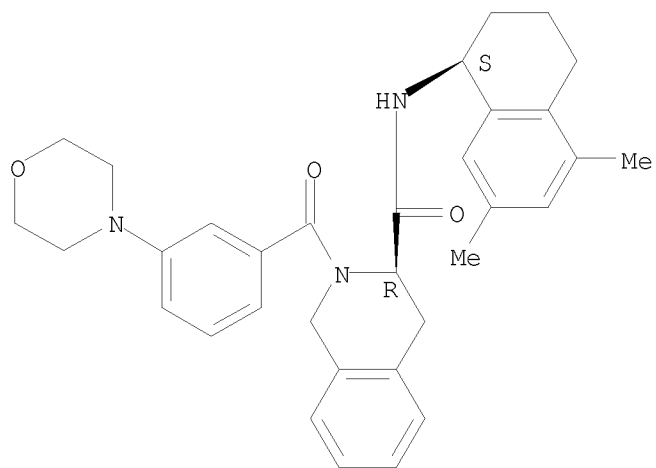
RN 215315-37-0 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[(1R)-1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl]-, (3R)-rel- (CA
 INDEX NAME)

Relative stereochemistry.

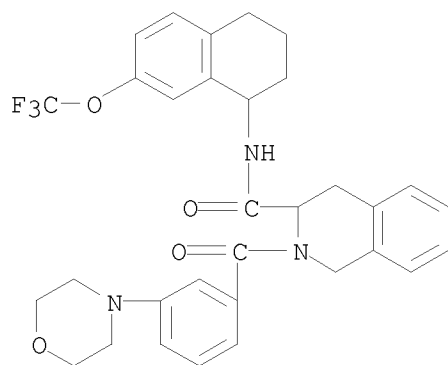


RN 215315-38-1 CAPLUS
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 N-[(1R)-1,2,3,4-tetrahydro-5,7-dimethyl-1-naphthalenyl]-, (3S)-rel- (CA
 INDEX NAME)

Relative stereochemistry.

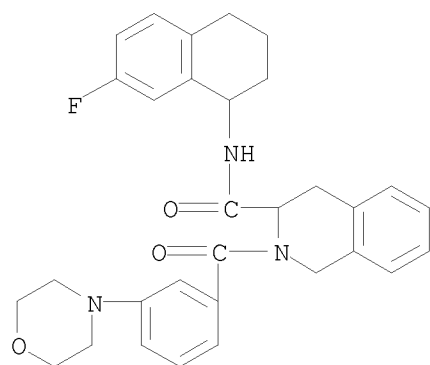


RN 215315-39-2 CAPLUS
 CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]-
 N-[1,2,3,4-tetrahydro-7-(trifluoromethoxy)-1-naphthalenyl]- (CA INDEX
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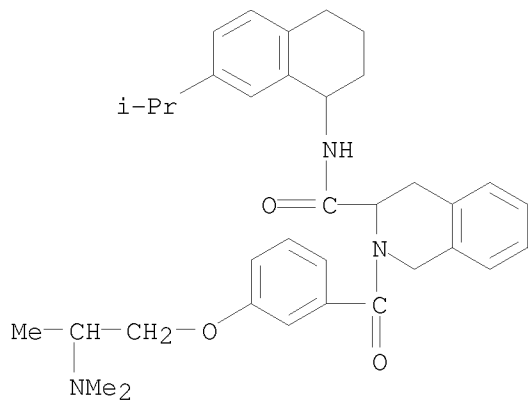
RN 215315-40-5 CAPLUS

CN 3-Isoquinolinecarboxamide, N-(7-fluoro-1,2,3,4-tetrahydro-1-naphthalenyl)-1,2,3,4-tetrahydro-2-[3-(4-morpholinyl)benzoyl]- (CA INDEX NAME)



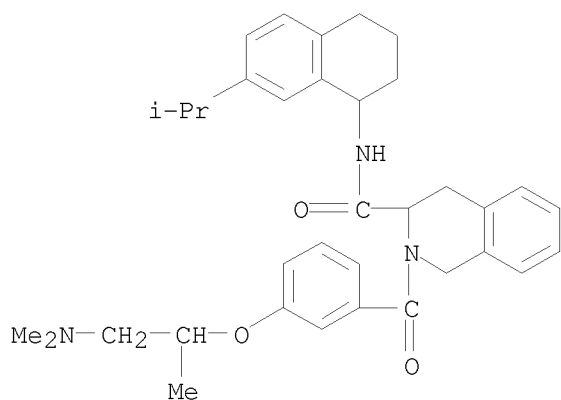
RN 215315-41-6 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)propoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]- (CA INDEX NAME)



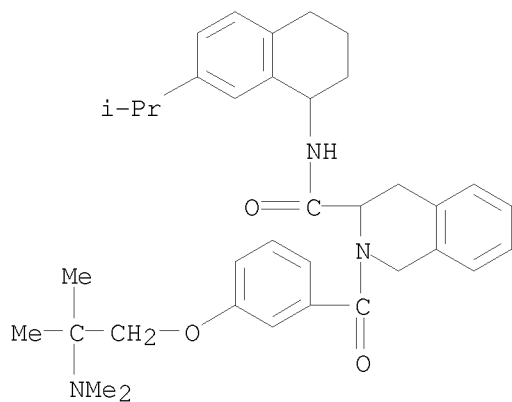
RN 215315-42-7 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)-1-methylethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-(CA INDEX NAME)



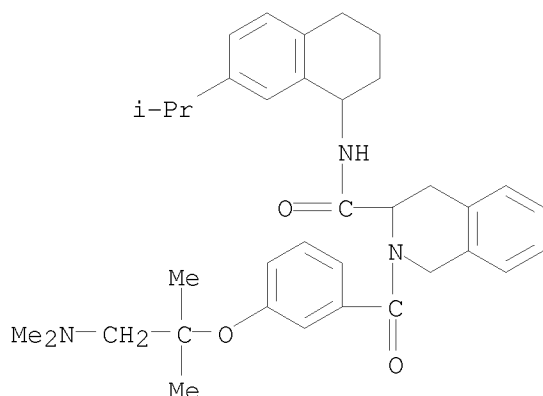
RN 215315-43-8 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)-2-methylpropoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-(CA INDEX NAME)



RN 215315-44-9 CAPLUS

CN 3-Isoquinolinecarboxamide, 2-[3-[2-(dimethylamino)-1,1-dimethylethoxy]benzoyl]-1,2,3,4-tetrahydro-N-[1,2,3,4-tetrahydro-7-(1-methylethyl)-1-naphthalenyl]-(CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:390174 CAPLUS

DOCUMENT NUMBER: 127:95591

ORIGINAL REFERENCE NO.: 127:18412h, 18413a

TITLE: Incorporation of conformationally constrained phenylalanine derivatives Tic, Sic, Hic and Nic into a cholecystokinin-B/gastrin receptor antagonist

AUTHOR(S) : Gibson, Susan E.; Guillo, Nathalie; Kalindjian, S. Barret; Tozer, Matthew J.

CORPORATE SOURCE: Dep. Chem., Imperial Coll. Sci., Technol. Med.,
London, SW7 2AY, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (1997),
7(10), 1289-1292

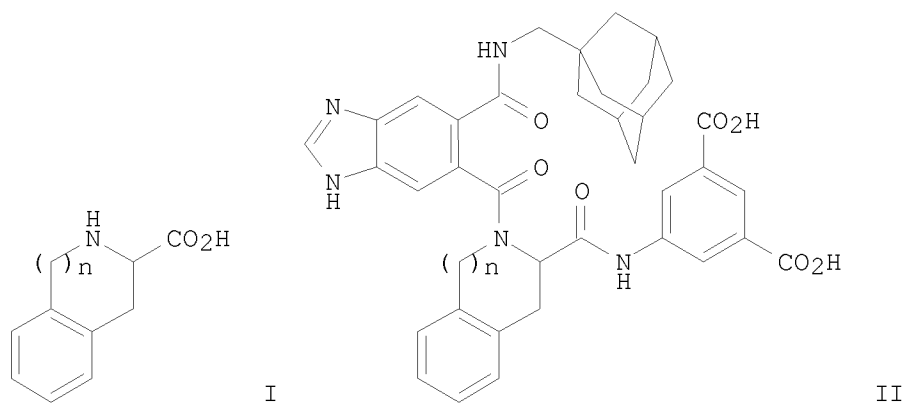
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



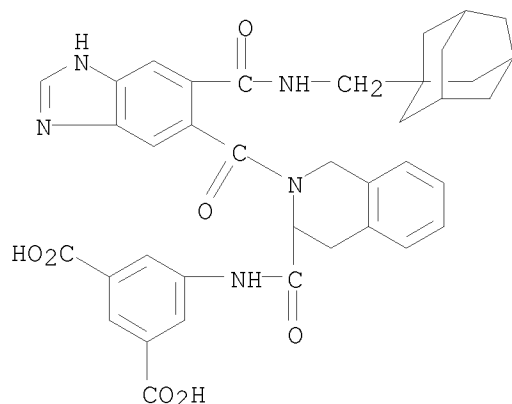
AB The preparation and biol. properties of a conformationally constrained series of cholecystokinin-B/gastrin receptor ligands containing constrained phenylalanine analogs I (n = 1-4) are described. The 9-membered ring derivative II (n = 4) was as active at these receptors as an unconstrained phenylalanine analog.

IT 192134-02-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(incorporation of conformationally constrained phenylalanine derivs. into cholecystokinin-B/gastrin receptor antagonist)

RN 192134-02-4 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[[[1,2,3,4-tetrahydro-2-[[5-[[[(tricyclo[3.3.1.1^{3,7}]dec-1-ylmethyl)amino]carbonyl]-1H-benzimidazol-6-yl]carbonyl]-3-isoquinoliny]carbonyl]amino]- (CA INDEX NAME)

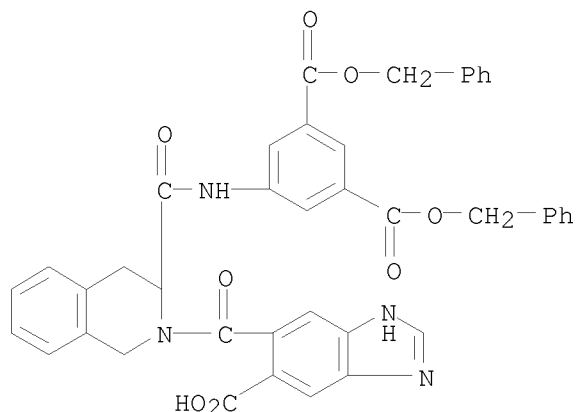


IT 192133-93-0P 192133-97-4P

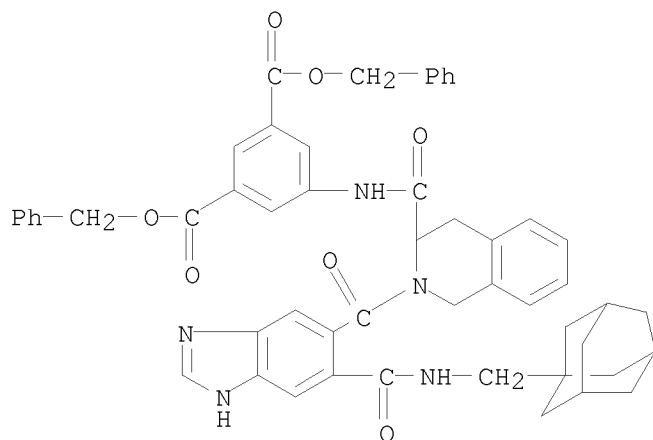
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(incorporation of conformationally constrained phenylalanine derivs. into cholecystokinin-B/gastrin receptor antagonist)

RN 192133-93-0 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[[[2-[(6-carboxy-1H-benzimidazol-5-yl)carbonyl]-1,2,3,4-tetrahydro-3-isoquinoliny]carbonyl]amino]-, 1,3-bis(phenylmethyl) ester (CA INDEX NAME)



RN 192133-97-4 CAPLUS
 CN 1,3-Benzenedicarboxylic acid, 5-[[[1,2,3,4-tetrahydro-2-[[5-[[[(tricyclo[3.3.1.1.3,7]dec-1-ylmethyl)amino]carbonyl]-1H-benzimidazol-6-yl]carbonyl]-3-isoquinolinyl]carbonyl]amino]-, 1,3-bis(phenylmethyl) ester (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

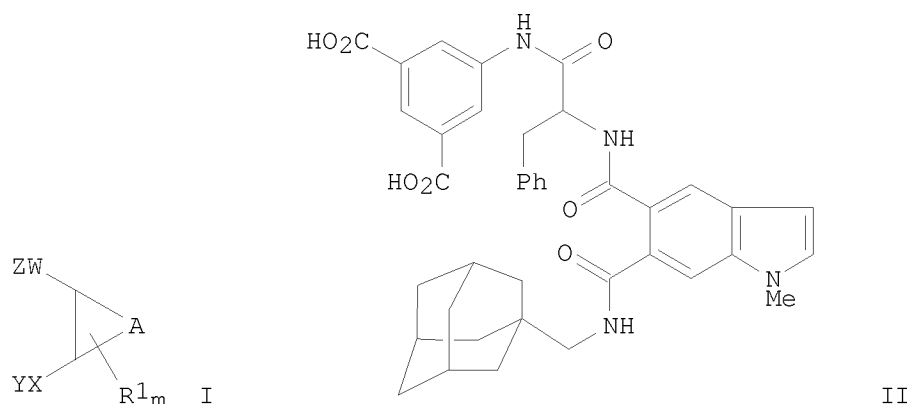
L4 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1995:801429 CAPLUS
 DOCUMENT NUMBER: 123:256711
 ORIGINAL REFERENCE NO.: 123:45919a,45922a
 TITLE: Preparation of gastrin and CCK receptor ligands
 INVENTOR(S): Kalindjian, Sarkis Barret; Steel, Katherine Isobel Mary; Pether, Michael John; Davies, Jonathan Michael Richard; Low, Caroline Minli Rachel; Hudson, Martin Lyn; Buck, Ildiko Maria; McDonald, Iain Mair; Dunstone, David John; Tozer, Matthew John
 PATENT ASSIGNEE(S): James Black Foundation Ltd., UK

SOURCE: PCT Int. Appl., 124 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9504720	A2	19950216	WO 1994-GB1741	19940809
WO 9504720	A3	19950803		
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2167154	A1	19950216	CA 1994-2167154	19940809
AU 9473478	A	19950228	AU 1994-73478	19940809
AU 682051	B2	19970918		
EP 720601	A1	19960710	EP 1994-922318	19940809
EP 720601	B1	20001025		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09502430	T	19970311	JP 1995-506306	19940809
JP 3980052	B2	20070919		
HU 75301	A2	19970528	HU 1996-70	19940809
HU 222178	B1	20030428		
AT 197146	T	20001115	AT 1994-922318	19940809
ES 2152989	T3	20010216	ES 1994-922318	19940809
PT 720601	T	20010228	PT 1994-922318	19940809
PL 181782	B1	20010928	PL 1994-312960	19940809
ZA 9405998	A	19960212	ZA 1994-5998	19940810
GB 2290539	A	19960103	GB 1995-2503	19950209
WO 9532949	A1	19951207	WO 1995-GB1194	19950525
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9525342	A	19951221	AU 1995-25342	19950525
EP 763026	A1	19970319	EP 1995-919561	19950525
EP 763026	B1	20030326		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10504525	T	19980506	JP 1996-500483	19950525
AT 235470	T	20030415	AT 1995-919561	19950525
ZA 9504315	A	19961126	ZA 1995-4315	19950526
NO 9600488	A	19960315	NO 1996-488	19960206
NO 306945	B1	20000117		
FI 9600572	A	19960207	FI 1996-572	19960207
FI 115050	B1	20050228		
US 5795907	A	19980818	US 1996-583008	19960318
US 5912260	A	19990615	US 1996-737725	19961219
US 5919829	A	19990706	US 1998-64849	19980423
GR 3035100	T3	20010330	GR 2000-402788	20001218
PRIORITY APPLN. INFO.:			GB 1993-16608	A 19930810
			GB 1994-10688	A 19940527

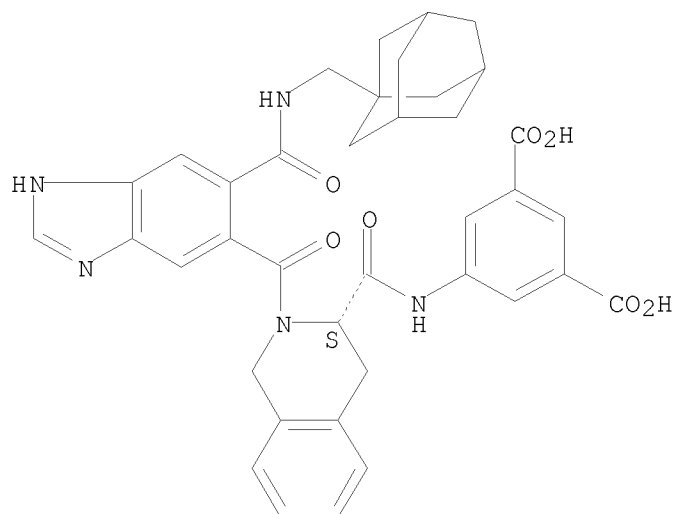
WO 1994-GB1741 W 19940809
 GB 1995-2503 A 19950209
 WO 1995-GB1194 W 19950525

OTHER SOURCE(S): CASREACT 123:256711; MARPAT 123:256711
 GI



- AB Title compds. [e.g. I; A = atoms to complete a bicyclic ring system; R₁ = halo, NH₂, cyano, OH, alkyl, CO₂H, etc.; 1 of X, W = CO and the other = CO, SO, SO₂; Y = NR₃R₄, hydrocarbyloxy, etc.; R₃ = H, hydrocarbyl, etc.; R₄ = H, alkyl, (un) esterified CH₂CO₂H; Z = OH, alkoxy, OPh, (un)substituted NH₂, NHZ₁R, etc.; R = H, cyano, alkyl, CH₂OH, CO₂H, etc.; Z₁ = alkylene; m = 0-6] were prepared Thus, 4-methylphthalic anhydride was converted in 6 steps to indole-5,6-dicarboxylic anhydride which was amidated by adamantane-1-methylamine and the product amidated by (S)-3,5-(PhH₂CO₂C)2C₆H₃NHCOCH(NH₂)CH₂Ph (preparation given) to give, in 2 addnl. steps, title compound (S)-II the di-N-methyl-D-glucamine salt of which had pK_i of 9.4 for binding at mouse cortex CCKB receptors in vitro.
- IT 167992-44-1P 167992-45-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of gastrin and CCK receptor ligands)
- RN 167992-44-1 CAPLUS
- CN 1,3-Benzenedicarboxylic acid, 5-[[[1,2,3,4-tetrahydro-2-[[6-[[[(tricyclo[3.3.1.1^{3,7}]dec-1-ylmethyl)amino]carbonyl]-1H-benzimidazol-5-yl]carbonyl]-3-isoquinolinyl]carbonyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

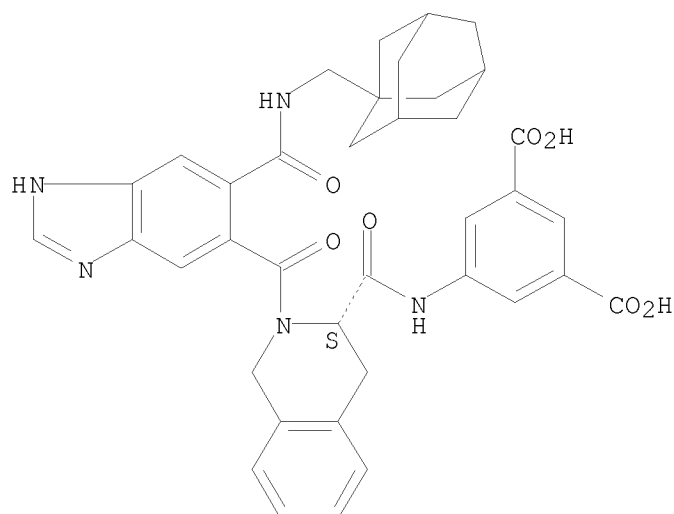


RN 167992-45-2 CAPLUS
 CN D-Glucitol, 1-deoxy-1-(methylamino)-, (S)-5-[[[1,2,3,4-tetrahydro-2-[[6-
 [[(tricyclo[3.3.1.1^{3,7}]dec-1-ylmethyl)amino]carbonyl]-1H-benzimidazol-5-
 yl]carbonyl]-3-isoquinoliny]carbonyl]amino]-1,3-benzenedicarboxylate
 (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 167992-44-1
 CMF C38 H37 N5 O7

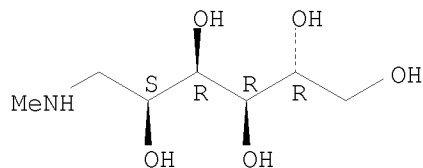
Absolute stereochemistry.



CM 2

CRN 6284-40-8
CMF C7 H17 N O5

Absolute stereochemistry.



L4 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:536786 CAPLUS

DOCUMENT NUMBER: 115:136786

ORIGINAL REFERENCE NO.: 115:23483a, 23486a

TITLE: Preparation of peptide p-pyridazinylanilides as cardiovascular agents.

INVENTOR(S): Bru-Magniez, Nicole; Nicolai, Eric; Teulon, Jean Marie

PATENT ASSIGNEE(S): Laboratoires UP SA S. A., Fr.

SOURCE: Fr. Demande, 73 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

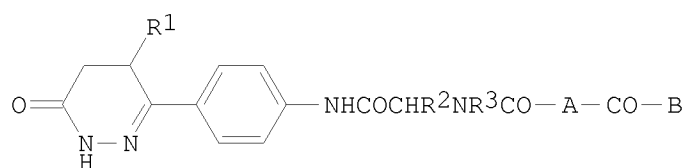
LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

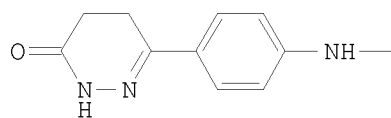
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2646853	A1	19901116	FR 1989-6066	19890509
PRIORITY APPLN. INFO.:			FR 1989-6066	19890509
OTHER SOURCE(S):	CASREACT	115:136786; MARPAT	115:136786	

GI



I



Q

AB The title compds. I [R1 = H, alkyl; R2 = H, alkyl, aralkyl, halo, OH, etc.; R3 = H, alkyl; or R2R3 = CH2(XH2)nCH2; n = 1-4; A = pyrrolidinediyl, etc.; B = CHR4X; R4 = H, alkyl, amino; X = CH2SH, CH2SAc, etc.] and their pharmaceutically acceptable salts, useful as cardiotonics, vasodilators, blood platelet aggregation inhibitors, and angiotensin converting enzyme inhibitors, were prepared Amidation of Z-Pro-Phe-OH (Z = PhCH2O2C) with

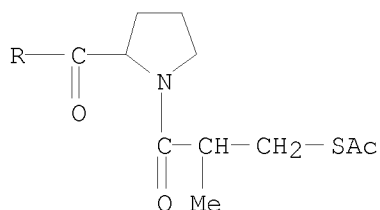
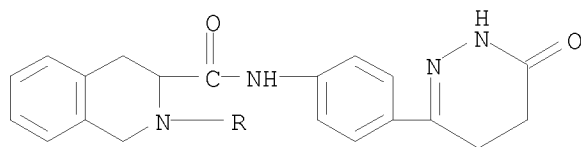
pyridazinylaniline QH (preparation given), the resulting dipeptide amide Z-Pro-Phe-Q deprotected, and then condensed with AcSCH₂CHMeCOCl in CH₂Cl₂ containing Et₃N to give the title compound AcSCH₂CHMeCO-Pro-Phe-Q (II). In an in vitro experiment using guinea pig heart, II at 7.9 + 10⁻⁶ M effected 50% of the maximum inotropic augmentation.

IT 135836-31-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as cardiovascular agent)

RN 135836-31-6 CAPLUS

CN Ethanethioic acid, S-[3-[2-[[3,4-dihydro-3-[[[4-(1,4,5,6-tetrahydro-6-oxo-3-pyridazinyl)phenyl]amino]carbonyl]-2(1H)-isoquinolinyl]carbonyl]-1-pyrrolidinyl]-2-methyl-3-oxopropyl] ester, [3S-[2[R*(R*)],3R*]]- (9CI)
(CA INDEX NAME)



L4 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:488188 CAPLUS

DOCUMENT NUMBER: 109:88188

ORIGINAL REFERENCE NO.: 109:14627a,14630a

TITLE: Preparation of cyclic α -iminocarboxylic acid anilides, as herbicides

INVENTOR(S): Frey, Michael; Erhardt, Heinz; Mildenberger, Hilmar; Bauer, Klaus; Bieringer, Herman

PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 11 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

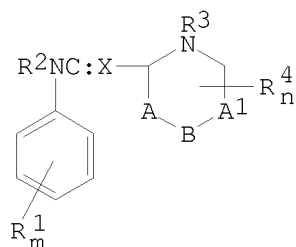
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3636278	A1	19880505	DE 1986-3636278	19861024
EP 264865	A2	19880427	EP 1987-115217	19871017

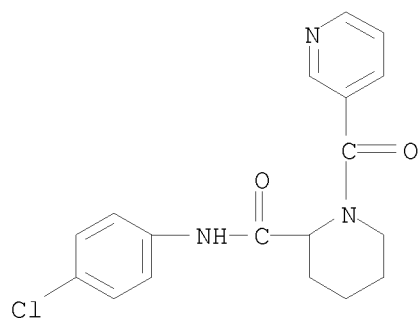
R: AT, BE, CH, DE, FR, GB, GR, IT, LI, LU, NL, SE

DD 262573	A5	19881207	DD 1987-308189	19871022
AU 8780075	A	19880428	AU 1987-80075	19871023
JP 63115861	A	19880520	JP 1987-266684	19871023
BR 8705695	A	19880531	BR 1987-5695	19871023
ZA 8707974	A	19880629	ZA 1987-7974	19871023
HU 47907	A2	19890428	HU 1987-4753	19871023
PRIORITY APPLN. INFO.:			DE 1986-3636278	A 19861024
OTHER SOURCE(S):		CASREACT 109:88188; MARPAT 109:88188		
GI				

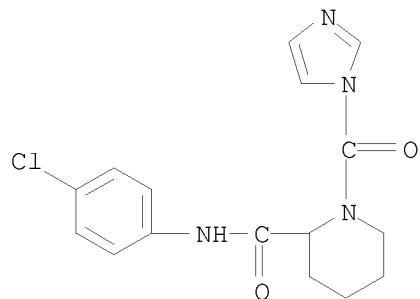


I

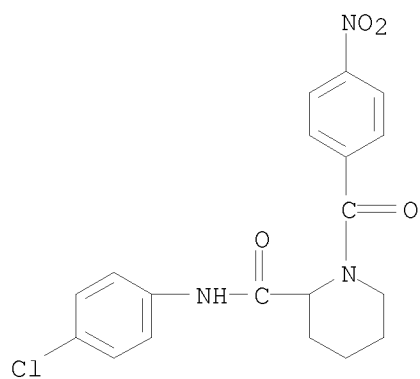
- AB The title compds. I [A, A1 = CH2, S, SO, SO2, CHR4, CR24; B = O, S, SO, SO2, CH2, CHR4 CR24, NR5, NCXR5, NCX2R5; X = O, S; R1 = alkyl, halo, NO2, alkoxy, etc.; R2 = H, alkyl; R3 = H, alkyl, cycloalkyl, haloalkyl, alkoxy, etc.; R4 = R5, CXR5, CX2R5; R5 = (un)substituted alkyl, Ph or benzyl; m = 0, 1-5; n = 0, 1-3] are prepared as herbicides. A solution of ClCO2 in toluene was added to a solution of piperidine-2-carboxylic acid 2-chloro-4-fluoro-5-methoxyanilide and Et3N in toluene, to give 1-(ethoxycarbonyl)piperidine-2-carboxylic acid 2-fluoro-4-chloro-5-methoxyanilide. I has high herbicidal activity, both pre- and postemergence, against unspecified weeds, in pot expts.
- IT 67691-53-6P 115687-84-8P 115687-85-9P
115687-86-0P 115687-87-1P 115710-57-1P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)
- RN 67691-53-6 CAPLUS
- CN 2-Piperidinecarboxamide, N-(4-chlorophenyl)-1-(3-pyridinylcarbonyl)- (CA INDEX NAME)



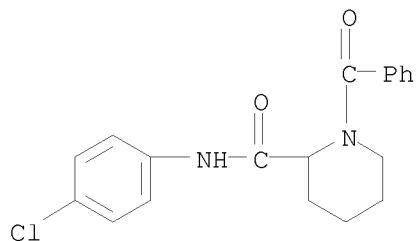
RN 115687-84-8 CAPLUS
 CN 2-Piperidinecarboxamide, N-(4-chlorophenyl)-1-(1H-imidazol-1-ylcarbonyl)-
 (CA INDEX NAME)



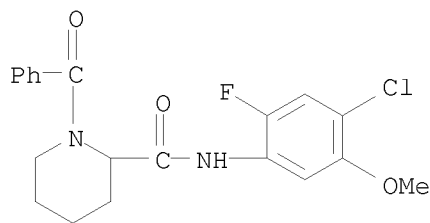
RN 115687-85-9 CAPLUS
 CN 2-Piperidinecarboxamide, N-(4-chlorophenyl)-1-(4-nitrobenzoyl)- (CA INDEX
 NAME)



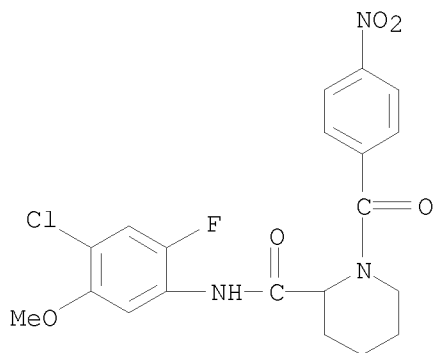
RN 115687-86-0 CAPLUS
 CN 2-Piperidinecarboxamide, 1-benzoyl-N-(4-chlorophenyl)- (CA INDEX NAME)



RN 115687-87-1 CAPLUS
 CN 2-Piperidinecarboxamide, 1-benzoyl-N-(4-chloro-2-fluoro-5-methoxyphenyl)-
 (CA INDEX NAME)



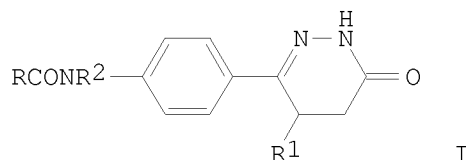
RN 115710-57-1 CAPLUS
 CN 2-Piperidinecarboxamide, N-(4-chloro-2-fluoro-5-methoxyphenyl)-1-(4-nitrobenzoyl)-
 (CA INDEX NAME)



L4 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1983:488219 CAPLUS
 DOCUMENT NUMBER: 99:88219
 ORIGINAL REFERENCE NO.: 99:13613a,13616a
 TITLE: Pyridazinone derivatives
 INVENTOR(S): Katakami, Tsutomu; Fukazawa, Nobuyuki; Iizuka, Hajime;
 Nishina, Takashi; Kamiya, Joji; Tanaka, Yasuhito;
 Nakano, Takuo
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc. , Japan

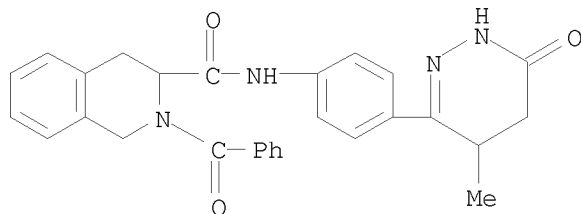
SOURCE: PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8301447	A1	19830428	WO 1982-JP415	19821020
W: US				
RW: DE, FR, GB				
JP 58069867	A	19830426	JP 1981-166437	19811020
JP 60058234	B	19851219		
JP 58069868	A	19830426	JP 1981-166438	19811020
JP 05026780	B	19930419		
JP 58113179	A	19830705	JP 1981-209937	19811228
JP 03053303	B	19910814		
EP 107735	A1	19840509	EP 1982-903181	19821020
EP 107735	B1	19881019		
R: DE, FR, GB				
US 4639451	A	19870127	US 1983-504039	19830603
US 4965263	A	19901023	US 1989-310505	19890214
PRIORITY APPLN. INFO.:			JP 1981-166437	A 19811020
			JP 1981-166438	A 19811020
			JP 1981-209937	A 19811228
			WO 1982-JP415	W 19821020
			US 1983-504039	A3 19830603
			US 1986-913687	B1 19860925
OTHER SOURCE(S):		CASREACT 99:88219		
GI				



- AB The title compds. I [R = (substituted) aryl, etc; R1, R2 = H, alkyl] were prepared by acylation of the appropriate (aminophenyl)pyridazinones with RCO2H or their reactive derivs. Thus, stirring a mixture of 1.2 g salicylic chloride, 1.0 g 6-(p-aminophenyl)-5-methyl-4,5-dihydro-3(2H)-pyridazinone, and 10 mL benzene at 50° for 6 h gave 750 mg I (R = o-HOC6H4, R1 = Me, R2 = H). I at 4 mg/kg had antihypertensive and blood platelet aggregation-inhibiting activities comparable to those of hydralazine in rats.
- IT 86800-46-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation and pharmacol. activities of)

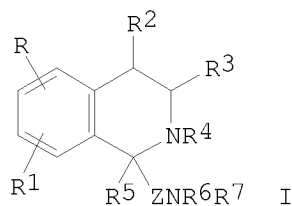
RN 86800-46-6 CAPLUS
 CN 3-Isoquinolinecarboxamide, 2-benzoyl-1,2,3,4-tetrahydro-N-[4-(1,4,5,6-tetrahydro-4-methyl-6-oxo-3-pyridazinyl)phenyl]- (CA INDEX NAME)



L4 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1983:89195 CAPLUS
 DOCUMENT NUMBER: 98:89195
 ORIGINAL REFERENCE NO.: 98:13611a,13614a
 TITLE: Isoquinoline derivatives
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57139066	A	19820827	JP 1981-24812	19810220
PRIORITY APPLN. INFO.:			JP 1981-24812	19810220
OTHER SOURCE(S):	CASREACT	98:89195		

GI



AB Thirty-seven isoquinoline derivs. I (R, R1 = H, OH, acyloxy, alkoxy; R2, R3 = H; R2 and R3 may be a bond; R4 = H, acyl; R5 = H; R4 and R5 may be a bond; R6 = H, alkyl; R7 = alkyl-substituted 5-membered N heterocyclic; Z = alkylene) were prepared by, e.g., reaction of RR1C6H3CH2CH2NH2 (II) with R6R7NZCHO (III). Antiulcer test data of I were shown. Thus, stirring a mixture of 2.15 g (1-methyl-1H-tetrazol-5-yl)aminoacetaldehyde di-Et acetal and 3 mL MeI in DMF with 0.57 g 65% NaH 2 h at 5° gave 2.18 g III di-Et acetal (R6 = Me, R7 = 1-methyl-1H-tetrazol-5-yl, Z = CH2) (IV). A mixture of 2.84 g IV, 4.6 g II.HCl (R, R1 = 3-,4-OH), and 0.9 mL concentrated HCl

in aqueous EtOH was stirred for 5 h at 90° to give 2.3 g I.HCl (R,R1 = 3-, 4-OH, R2 = R3 = R4 = R5 = H, R6 = Me, R7 = 1-methyl-1H-tetrazol-5-yl, Z = CH2).

IT 84641-15-6P 84641-16-7P 84641-34-9P
84641-35-0P

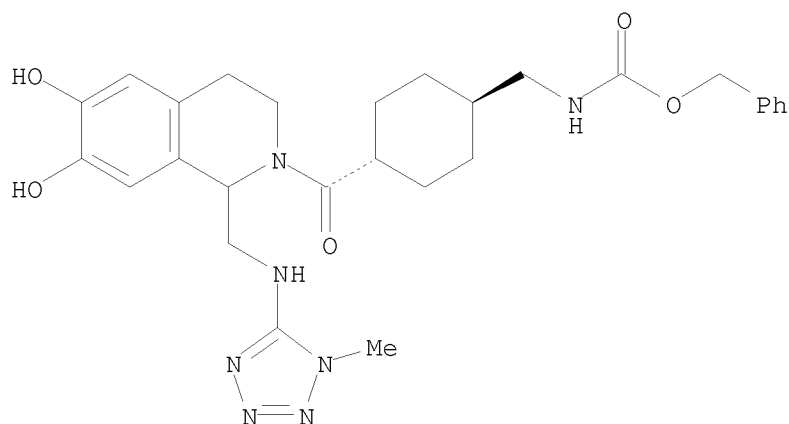
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antiulcer activity of)

RN 84641-15-6 CAPLUS

CN Carbamic acid, [[4-[[[3,4-dihydro-6,7-dihydroxy-1-[[[1-methyl-1H-tetrazol-5-yl)amino]methyl]-2(1H)-isoquinolinyl]carbonyl]cyclohexyl]methyl]-, phenylmethyl ester, trans- (9CI) (CA INDEX NAME)

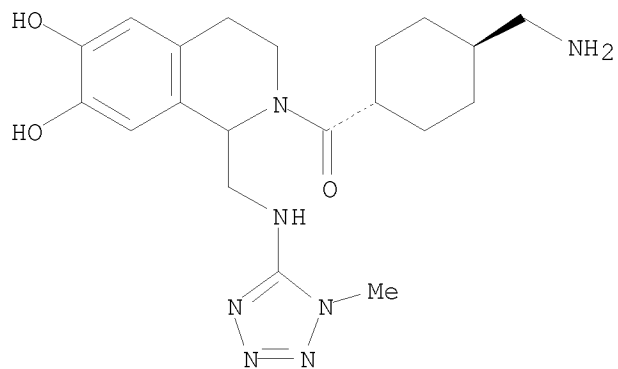
Relative stereochemistry.



RN 84641-16-7 CAPLUS

CN 6,7-Isoquinolinediol, 2-[[[4-(aminomethyl)cyclohexyl]carbonyl]-1,2,3,4-tetrahydro-1-[[[1-methyl-1H-tetrazol-5-yl)amino]methyl]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

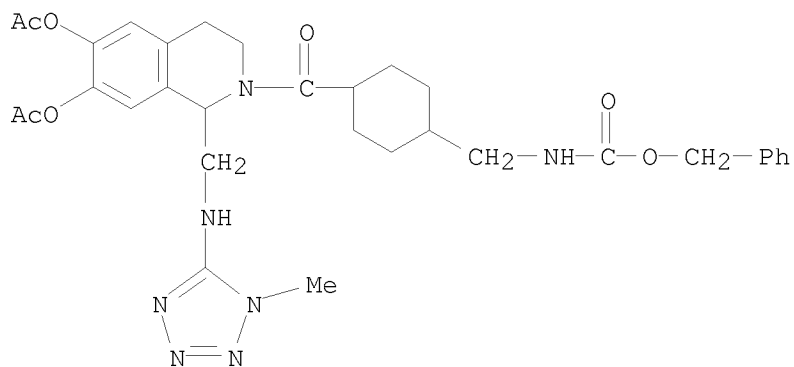
Relative stereochemistry.



● HCl

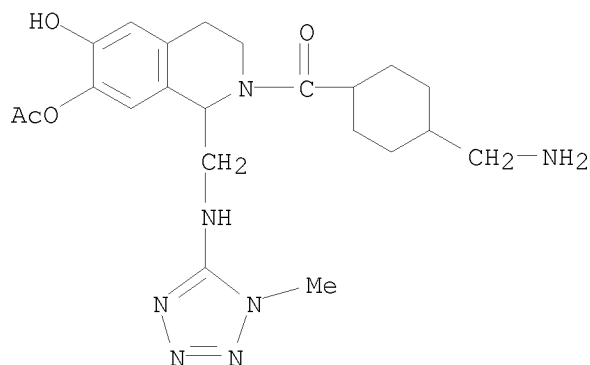
RN 84641-34-9 CAPLUS

CN Carbamic acid, [[4-[[6,7-bis(acetyloxy)-3,4-dihydro-1-[[1-methyl-1H-tetrazol-5-yl]amino]methyl]-2(1H)-isoquinoliny]carbonyl]cyclohexyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

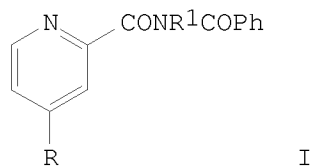


RN 84641-35-0 CAPLUS

CN 6,7-Isoquinolinediol, 2-[[4-(aminomethyl)cyclohexyl]carbonyl]-1,2,3,4-tetrahydro-1-[[1-methyl-1H-tetrazol-5-yl]amino]methyl]-, 7-acetate (9CI) (CA INDEX NAME)

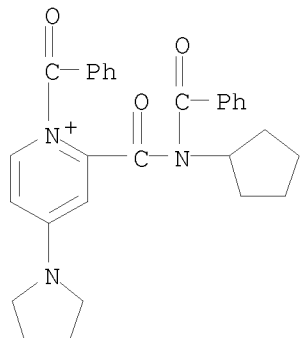


L4 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1982:598074 CAPLUS
 DOCUMENT NUMBER: 97:198074
 ORIGINAL REFERENCE NO.: 97:33173a,33176a
 TITLE: Studies of substituted N-benzoyl-2-pyridinecarboxamides. Reactions with acyl chlorides and other electrophiles
 AUTHOR(S): Moerkved, Eva H.
 CORPORATE SOURCE: Norw. Inst. Technol., Univ. Trondheim, Trondheim, N-7034, Norway
 SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1982), B36(2), 77-84
 CODEN: ACBOCV; ISSN: 0302-4369
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 97:198074
 GI



AB I (R = morpholino, R1 = Ph, 2-pyridyl, cyclopentyl) react as nucleophiles with PhCOCl to give adducts which are stabilized by further addition of 1 mol. H2O. The adducts were also prepared by treating 4-morpholino-2-pyridinecarboxamides with 2 mol. equivalent PhCOCl and Et3N. I (R = 1-pyrrolidinyl, R1 = 2-pyridyl, cyclopentyl) gave less stable adducts with PhCOCl, whereas N-benzoyl-2-pyridinecarboxamides were unreactive. I gave stable adducts with ClCH2SO3Me, AcCl, and p-MeC6H4SO3H, but were unreactive toward MeI, Ph2NCOCl, and Ac2O.
 IT 82776-80-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 82776-80-5 CAPLUS

CN Pyridinium, 1-benzoyl-2-[(benzoylcyclopentylamino)carbonyl]-4-(1-pyrrolidinyl)-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L4 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:529406 CAPLUS

DOCUMENT NUMBER: 89:129406

ORIGINAL REFERENCE NO.: 89:20021a,20024a

TITLE: N-Acylpiperidinecarboxanilide derivatives

INVENTOR(S): Kinoshita, Sachihiko; Kobayashi, Michihiro; Akabane, Kenji; Kamijo, Yukio; Yamamoto, Ryoji; Ajisawa, Yukiyo

PATENT ASSIGNEE(S): Kissei Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

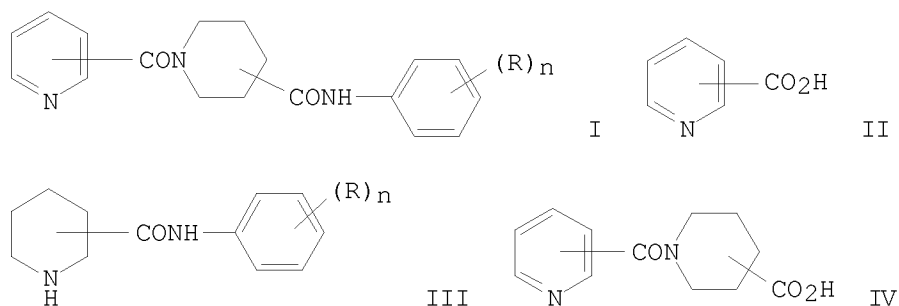
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 53031669	A	19780325	JP 1976-105742	19760906
PRIORITY APPLN. INFO.: GI			JP 1976-105742	A 19760906

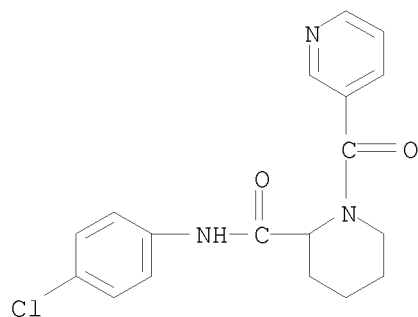


AB Eleven title derivs. I (R = alkyl, alkoxy, halo; n = 1-2) were prepared by reaction of II with III or IV with H₂NC₆H₅-nR_n. I are useful as anti-ulcer agents (no data). Thus, 20 mL SOCl₂ was added to 3.2 g N-nicotinoylisonipecotic acid to give the chloride HCl salt, which was refluxed with 1.7 g 2,6-xylydine in pyridine-C₆H₆ 10 h to give 2.9 g N-nicotinoylisonipecotic acid 2,6-dimethylanilide.

IT 67691-53-6P 67691-54-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

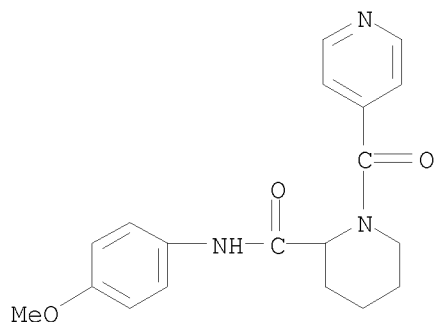
RN 67691-53-6 CAPLUS

CN 2-Piperidinecarboxamide, N-(4-chlorophenyl)-1-(3-pyridinylcarbonyl)- (CA INDEX NAME)

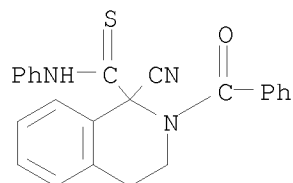


RN 67691-54-7 CAPLUS

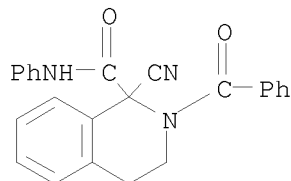
CN 2-Piperidinecarboxamide, N-(4-methoxyphenyl)-1-(4-pyridinylcarbonyl)- (CA INDEX NAME)



L4 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1972:461757 CAPLUS
 DOCUMENT NUMBER: 77:61757
 ORIGINAL REFERENCE NO.: 77:10215a,10218a
 TITLE: Alkylation, acylation, and reduction studies on
 1-cyano-1,2-dihydro- and -1,2,3,4-
 tetrahydroisoquinoline derivatives
 AUTHOR(S): Boehme, Horst; Stoecker, Klaus Peter
 CORPORATE SOURCE: Pharm.-Chem. Inst., Univ. Marburg, Marburg/L., Fed.
 Rep. Ger.
 SOURCE: Chemische Berichte (1972), 105(5), 1578-85
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI For diagram(s), see printed CA Issue.
 AB Successive treatment of 2-benzoyl-1-cyano-1,2,3,4-tetrahydroisoquinoline
 (I) with NaH in DMF and with alkyl or acyl halides gave the corresponding
 1-alkyl- or 1-acyl-1-cyano-1,2,3,4-tetrahydroisoquinolines (II), resp.
 Thioacylation and cyanoethylation of I with PhNCS and CH₂:CHCN, resp.,
 also took place in 1-position. Reduction of 2-alkyl-1-cyano-1,2-
 dihydroisoquinolines with LiAlH₄ gave 2-alkyl-1,2-dihydro-isoquinolines
 (III).
 IT 37039-23-9P 37039-43-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 37039-23-9 CAPLUS
 CN 1-Isoquinolinecarbothioamide, 2-benzoyl-1-cyano-1,2,3,4-tetrahydro-N-
 phenyl- (CA INDEX NAME)



RN 37039-43-3 CAPLUS
 CN 1-Isoquinolinecarboxamide, 2-benzoyl-1-cyano-1,2,3,4-tetrahydro-N-phenyl-
 (CA INDEX NAME)



L4 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:454417 CAPLUS

DOCUMENT NUMBER: 67:54417

ORIGINAL REFERENCE NO.: 67:10267a,10270a

TITLE: Optically active amino acids. XIII. Racemization of N-benzoylanilides of optically active proline and pipecolic acid

AUTHOR(S): Kunieda, Takehisa; Koga, Kenji; Yamada, Shunichi

CORPORATE SOURCE: Univ. Tokyo, Tokyo, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1967), 15(3), 350-1

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB CA 67: 22124d. Effect of ring size on rate of racemization of monocyclic α -amino acid derivs. such as (-)-1-benzoyl-2-pyrrolidinecarboxanilide (I) and (+)-1-benzoyl-2-piperidinecarboxanilide (II) is studied. N,N'-Dicyclohexylcarbodiimide (2 g.) was added to a solution of 2.1 g. N-benzoyl-L-proline (III) and 0.93 g. PhNH₂ in 45 ml. CH₂Cl₂, stirred at room temperature 3.5 hrs., clarified by filtration, washed with aqueous NaHCO₃ solution, and concentrated to give 1.7 g. I, m. 185-6°, [α]_D²⁰ -115.6° (c 1.6, EtOH). A mixture of 6.57 g. III and 3.03 g. Et₃N in 120 ml. absolute PhMe at -7 to -5° was treated with 3.26 g. ClCO₂Et, kept at -5° for 25 min., treated with 2.8 g. PhNH₂, allowed to stand overnight, clarified by filtration, washed with dilute HCl and aqueous NaHCO₃ solution, and concentrated to give 5.5 g. I.

II, m. 167-9°, [α]_D²⁰ 55.8° (c 1.04, EtOH), was similarly prepared Their rate of racemization was measured polarimetrically in Me₂SO solution at 40 ± 0.5°, using 3 moles of NaOEt as a base to show that I racemized 6 times faster than II.

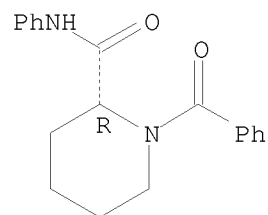
IT 15150-61-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(racemization of, kinetics of)

RN 15150-61-5 CAPLUS

CN Pipecolanilide, 1-benzoyl-, D- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



=> log h

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
197.64	378.51

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-28.80	-28.80

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 19:05:14 ON 14 SEP 2008